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Title: **USER'S MANUAL, VERSION 2.0 FOR MONTEBURNS, VERSION 5B**

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Los Alamos
NATIONAL LABORATORY

User's Manual, Version 2.0

for

Monteburns, Version 1.0

September 1, 1999

by

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FOR

MONTEBURNS, VERSION 1.0

by

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ABSTRACT

Monteburns is a fully automated tool that links the Monte Carlo transport code MCNP with the radioactive decay and burnup code ORIGEN2. *Monteburns* produces a large number of criticality and burnup results based on various material feed/removal specifications, power(s), and time intervals. The program processes input from the user that specifies the system geometry, initial material compositions, feed/removal specifications, and other code-specific parameters. Various results from MCNP, ORIGEN2, and other calculations are then output successively as the code runs. The principle function of *monteburns* is to transfer one-group cross-section and flux values from MCNP to ORIGEN2, and then transfer the resulting material compositions (after irradiation and/or decay) from ORIGEN2 back to MCNP in a repeated, cyclic fashion. The basic requirement of the code is that the user have a working MCNP input file and other input parameters; all interaction with ORIGEN2 and other calculations are performed by *monteburns*.

This report serves as a user's manual for *monteburns*. It describes how the code functions, what input the user must provide, and the calculations performed by the code. It also presents the format required for input files, as well as samples of these files. *Monteburns* is still in a developmental stage; thus, additions and/or changes may be made over time, and the user's manual will change as well. This is the second version of the user's manual (valid for *monteburns* previous version 5B, now known officially as Version 1.0); users should contact the authors to inquire if a more recent version is available (Note: for versions of *monteburns* before and including 4B, users should see the first version of the user's manual).

1.0. INTRODUCTION

As computational power continues to increase, it becomes more practical to utilize Monte Carlo methods to perform burnup calculations. *Monteburns* was designed to link the Monte Carlo N-Particle Transport Code (Ref. 1) MCNP and the radioactive decay and burnup code ORIGEN2 (Ref. 2). The primary function of MCNP is to calculate one-group cross-sections and fluxes that are used by ORIGEN2 in burnup calculations as well as provide criticality and neutron economy information if requested. After performing burnup calculations using ORIGEN2, *monteburns* passes isotopic compositions of materials back to MCNP to begin another burnup cycle.

Monteburns consists of a Perl script file that executes MCNP, ORIGEN2, and the FORTRAN77 code *monteb.f*. *Monteburns.pl* and *monteb.f* manipulate the input and output from MCNP and ORIGEN2 to form a completely automated burnup tool. The input to *monteburns* begins with a working MCNP input file, and its format does not have to be specific. Other input includes material feed and removal information, and other code-specific variables used to perform burnup calculations in ORIGEN2 concurrently with flux/cross-section calculations in MCNP. Final results are reported as a combination of the output from the aforementioned codes. The name *monteburns* was chosen because it is a **Monte** Carlo **burn**up tool.

2.0. REQUIRED USER TRAINING AND/OR BACKGROUND

To run *monteburns*, a user currently MUST have

- access to a UNIX, PC, or VMS operating system,
- working versions of MCNP and ORIGEN2 and the corresponding cross-section sets and ORIGEN2 decay information,
- a sufficient understanding of MCNP to create a **working** MCNP input file with desired parameters,
- the ability to compile and/or execute a FORTRAN77 program, and
- the ability to execute a Perl script file.†

MCNP is a trademark of Los Alamos National Laboratory and is available through the Radiation Safety Information Computational Center (RSICC) as code CCC-660.

ORIGEN2 is a popular radioactive decay and buildup code produced by Oak Ridge National Laboratory and distributed by the Radiation Safety Information Computational Center as code CCC-371.

† More information about the Perl language can be found at www.perl.com. Most versions of Perl can then be downloaded from there or www.activestate.com.

3.0. DESCRIPTION OF MONTEBURNS

Monteburns consists of a Perl script file that frequently interacts with a FORTRAN77 program, *monteb.f*. It is designed to link the Monte Carlo transport code MCNP with the radioactive decay and burnup code ORIGEN2. *Monteburns* produces a large number of criticality and burnup results based on various material feed / removal specifications, power(s), and time intervals. The program processes input from the user that specifies the system geometry, initial material compositions, feed / removal specifications, and other code-specific parameters. Various results from MCNP, ORIGEN2, and other calculations are then output successively as the code runs.

Monteburns performs one or more MCNP and ORIGEN2 runs for each user-specified time step. The number of MCNP / ORIGEN2 runs per time step is specified by the user (whereas multiple runs per time step increase accuracy, they also significantly increase execution time). The user can also specify continuous or discrete (all at one time) material feed and / or removal at each time step. The results obtained from *monteburns* are more accurate if long irradiation periods are broken up into smaller lengths of time because the physics and composition of materials in the system may change significantly per unit time. The user can then specify that the time steps be divided into even smaller segments for use in ORIGEN2. This is desirable because smaller time steps often produce more accurate results than longer time steps in ORIGEN2 (especially at the beginning of a system's life) because of differences in computational techniques. In addition, there is virtually no penalty on execution time by using smaller time steps in ORIGEN2 because almost all of the execution time lies with MCNP.

3.1. Description of *Monteburns*

The primary way in which MCNP and ORIGEN2 interact through *monteburns* is that MCNP provides one-group microscopic cross-sections and fluxes to ORIGEN2 for burnup calculations. After ORIGEN2 and MCNP have been run, results for each burn step are written into output files, and the isotopic compositions obtained from ORIGEN2 are used to generate a new MCNP input file for the next burn step. This MCNP input file contains the adjusted composition and density of each material being analyzed. To increase the accuracy of the burnup calculation, a "predictor" step is used in which ORIGEN2 is run halfway through the designated burn step. One-group cross-sections are then calculated at the midpoint of the burn step by MCNP. This assumes that the isotopics of the system at the midpoint are a reasonable approximation of the isotopics over the entire burn step (actually it is only important that the neutron flux energy spectrum be representative of the entire burn step). The user must be aware of this assumption and consequently ensure that burn intervals are not too long. *Monteburns* prints out a neutron flux spectrum and the grams of a number of isotopes present for each predictor and each outer burn step in an output file; if there is a large difference between the predictor and the actual burn step, then a shorter burn time should be considered. After the predictor step is executed, then ORIGEN2 is reexecuted with the new one-group cross-sections

(see Section 4.2 for more information). Figure 1 shows how *monteburns* interacts with MCNP and ORIGEN2.

The other key factor in balancing accuracy with execution time is determining the number of isotopes for which one-group cross-sections should be calculated. For some isotopes it may be important to modify the one-group cross-section, whereas for others, the default ORIGEN2 value may be used with little effect on the solution. Thus, it would be inefficient to calculate a one-group cross-section for every isotope included in the associated MCNP libraries, although this can be done if desired. Isotopes are deemed "important" in two ways. The first way is to explicitly list an isotope in the *monteburns* input file; this insures that one-group cross-sections will be calculated for this isotope during each burn step (and that this isotope will be included in the primary *monteburns* output). The other way in which an isotope is deemed "important" is based on a user input variable called the "importance fraction" (see Section 3.4.6 and / or 4.2 for more information).

There are a number of elements in MCNP for which "natural" cross-sections exist. However, ORIGEN2 does not recognize natural elements, so *monteburns* contains data to break natural elements into individual isotopes. If a natural cross-section exists in the MCNP input file, *monteburns* separates this element into its isotopic components, and then ORIGEN2 burns these isotopes individually (with the default ORIGEN2 library cross-sections). After the ORIGEN2 burn, *monteburns* lumps them back into the common element for use in MCNP. Although this may not be completely correct because ORIGEN2 cross-sections are not modified by MCNP (i.e., and thus not fully representative of the material), it is dictated by the lack of MCNP

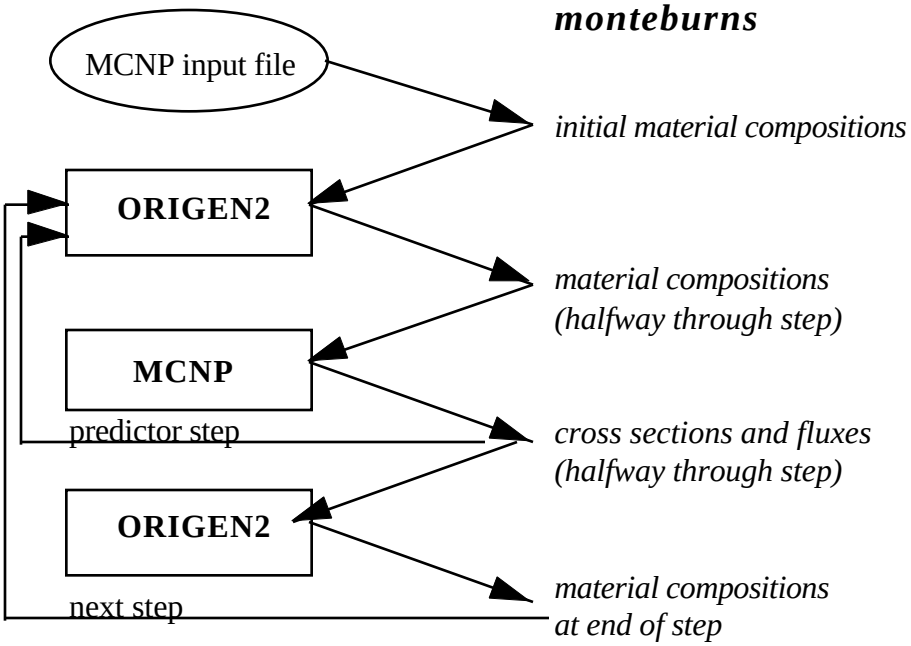

Fig. 1. Interaction of *Monteburns* with MCNP and ORIGEN2.

cross-sections for many individual isotopes. Whenever possible, it is recommended that the user specify the individual isotopes in the MCNP input file as opposed to using the natural element feature. This allows the isotopics of the element to change as the material burns; it also allows the one-group cross-sections to be modified if any of the isotopes are deemed "important."

The *monteburns code* does not currently perform any direct temperature-dependent calculations. The user is advised to use a code such as NJOY to process temperature-dependent cross-section libraries, which can then be used by MCNP to process temperature-dependent data. Additionally, *monteburns* is currently designed to work with MCNP4B, but it also works with MCNP4A and probably any earlier versions as well. *Monteburns* is also designed to work with either a "kcode" / "ksrc" (criticality) source definition in MCNP[1] or a "sdef" / "src" definition (for other types of transport calculations).

The FORTRAN77 program, *monteb.f*, which interacts with the Perl script file *monteburns.pl*, consists of 15 different parts, each of which performs a different function. These functions are displayed in the detailed flow chart of the Perl script file *monteburns.pl* in Fig. 2, where the numbers correspond to the list below.

1. Read input parameters
2. Create basic ORIGEN2 input files for each main burn step based on continuous feed / removal information
3. Put the user's MCNP input file into *monteburns* format
4. Create tally requests for MCNP
5. Write ORIGEN2 composition input file, separating natural elements into individual isotopes
6. Update the *monteburns* input file to indicate the current step number and to update the list of isotopes being tracked
7. Determine which material is located in each region
8. Add discrete feed to ORIGEN2 composition input file (if requested by the user)
9. Modify the previous MCNP input file with new material compositions
10. Modify ORIGEN2 input files for predictor steps to calculate compositions halfway through each burn step
11. Modify ORIGEN2 libraries with cross-sections calculated by MCNP and ORIGEN2 input files with fluxes from MCNP

[1] Versions of NJOY are available at the Radiation Safety Information Computational Center (RSICC) as codes PSR-171 and PSR-355.

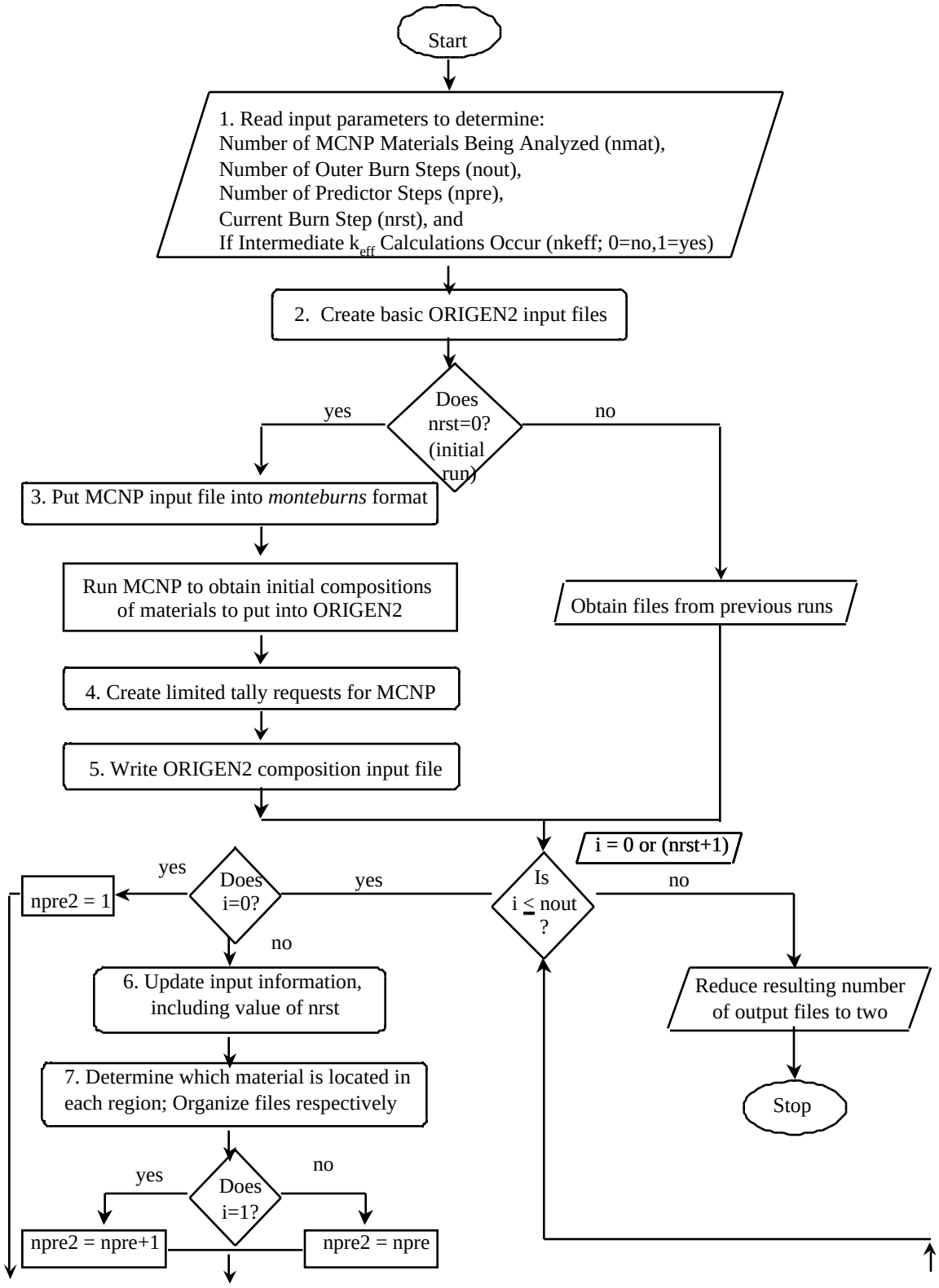

Fig. 2. *Monteburns* Flow Chart.

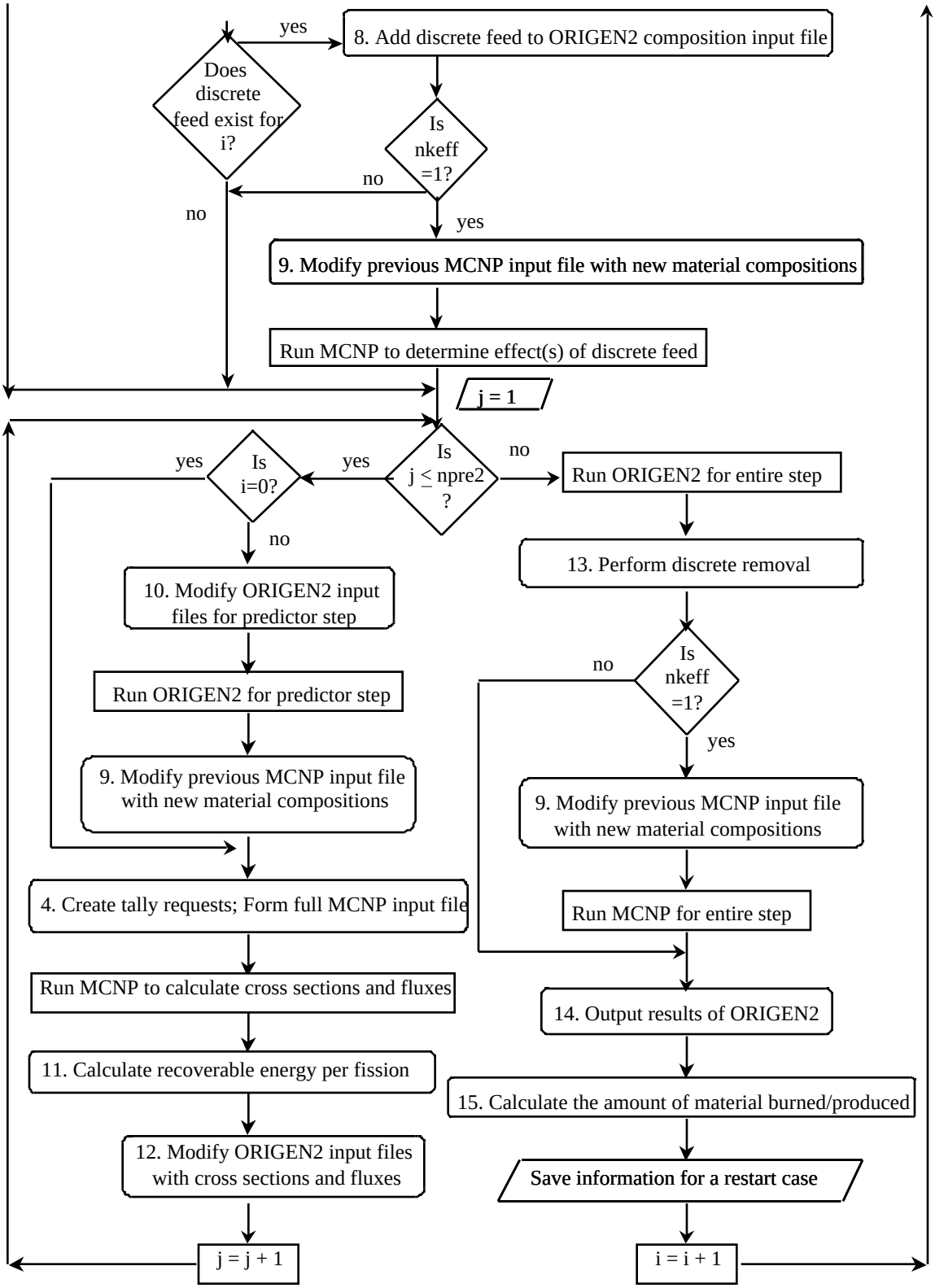

Fig. 2. *Monteburns* Flow Chart (cont).

12. Calculate the recoverable energy per fission based on the actinide distribution
13. Perform discrete removal in the ORIGEN2 composition input file
14. Output results of ORIGEN2
15. Calculate the amount of material burned and produced based on feed and inventory information

Table 1 describes the procedure followed in the execution of *monteburns* (excluding the file management steps) where *** is the base name of the various input files associated with *monteburns,* and # is the number of the current outer burn step. Note: VMS requires a *.dat extension on many files without extensions (primarily input and output from MCNP; therefore, these are included in parentheses where applicable. Table 2 then summarizes the function of each file used in *monteburns*.

Overall, *monteburns* acts as a pre- and postprocessor for both MCNP4B and ORIGEN2. Although the program is fully automated (except for the creation of input files), it is advised that the user be familiar with nuclear terminology, decay and burnup codes, and Monte Carlo codes such as MCNP to understand the output and to verify that the correct data were obtained.

3.2. MCNP Description

MCNP is a neutral particle transport code that uses the Monte Carlo technique. The Monte Carlo technique is a statistical method in which estimates for system characteristics are obtained through multiple computer simulations of the behavior of individual particles in a system. A Monte Carlo code generates such a statistical history for a particle based on random samples from probability distributions. These distributions are used in calculations to determine the type of interaction the particle undergoes at each point in its life, the resulting energy of the particle if it scatters, the number of particles that "leak" from the system because of geometry constraints, and the number of neutrons produced if the neutron causes a fission. The probability of the particle to behave in a certain manner (scatter, absorb, fission) can be obtained from the cross-section values of the material(s) with which the particle will interact. Thus, a Monte Carlo code can model the series of events that occur in the lives of a large number of particles to determine the flux of different types of particles in various regions in a system. These fluxes can then be used to tally a wide variety of information (reaction rates, heating rates, doses, etc.) for the system. Additionally, the value of the effective multiplication factor, k_{eff} , for a system (the ratio of the number neutrons in the system a particular time to the number of neutrons that existed in the previous generation) can be calculated using MCNP.

TABLE 1
PROCEDURE

Step	Process	Input[a]	Output[a]
1	Read input parameters from ***.inp input file (the primary *monteburns* input file – mb a)	***.inp = mb.inp tmpfile/params	mb.inp
2	Write natural element file (monteb e)	-	natelem
3	Create ORIGEN2 input files for each burn step (monteb 5)	***.feed = feed orig21/Decay.lib = ORIGEN2 decay lib. Orig**/^^^.lib = ORIGEN2 cross section library (**=ID#/^^^=name) tmpfile/param_$.#	tmpfile/TAPE5_$.I# TAPE9_0.INP mb9.txt mb9t_$.out tmpfile/params2
4	Modify MCNP input file to include commands specific to *monteburns* (monteb 1)	***	mbmc(.dat) mbmc.skl mat_$.inp mb*.txt (* = 1 to 17) mb*t_$.out (*=11,13)
5	Run the MCNP input processor on the initial MCNP input file to obtain the initial composition of the materials to be burned	*** = mbmc	mbmcm (optional) mbmco (.dat) mbmcr (.dat) mbmcs (.dat)
6	Create flux tally descriptions for MCNP input file (monteb 2)	mbmco(.dat)	tal2_$.inp mb6t_$.out
7	Write ORIGEN2 composition input file, fort.7 based on initial MCNP deck, and separate natural isotopes from non-actinides and other isotopes (monteb 4)	mbmco(.dat) mbxs.inp natelem	TAPE7_$.OUT mnat_$.tmp mcnp_$.inp
8	For a restart case, obtain files from previous runs	tmpfile/TAPE9_$.I# tmpfile/TAPE7_$.O# tmpfile/TAPE5_$.I# tmpfile/mbmc.# tmpfile/mbinp.#	TAPE9_$.INP TAPE7_$.OOU tmpfile/TAPE5_$.t# mbmc(.dat) mb.inp

[a]The following symbols apply for the table: # = number of the current outer burn step, $ = *monteburns* material number of current material being analyzed [may or may not be equal to MCNP material number (see Section 5.2 for more information)], *** = base names of files, and @ = the number 1–17.

TABLE 1 (cont)
PROCEDURE

Step	Process	Input[a]	Output[a]
9	Determine which material is in each region and organize files respectively	tmpfile / params2 feed tmpfile / TAPE5_$.t# mnat_$.tmp TAPE7_$.OUT	tmpfile / para3_$ tmpfile / TAPE5_$.I# mnat_$.tmp TAPE7_$.OUT
10	Rewrite input information, including number of outer steps currently being processed (monteb 9). Determine if discrete feed exists or not	***.inp = mb.inp tmpfile / param_$.#	mb.inp
11	Add discrete feed to ORIGEN2 composition input file (monteb b)	TAPE7_$.OUT tmpfile / params2 feed natelem	TAPE7_$.TMP tmpfile / param_$.# tape.tmp
12	Modify previous MCNP input file by adding discrete feed (monteb 7b)	TAPE7_$.OUT TAPE9_$.INP mbxs.inp mcnp_$.inp mnat_$.tmp	mb7_$.out mat_$.inp tmpfile / T9err_$.TXT mbmc.skl
13	Run MCNP to determine effect(s) of discrete feed	mbmc.skl mat_$.inp	mbmco(.dat)
14	Obtain criticality values from MCNP output file (monteb 6b)	mbmco(.dat) tmpfile / params2 feed	mb11_$.out
15	Output results (monteb 8b)	TAPE7_$.OUT	mb5.._$.out
16	Run ORIGEN2 for predictor step(s) (i.e., halfway through each step)	tmpfile / TAPE5_$.# = TAPE5_$.INP TAPE4_$.INP TAPE9_$.INP tmpfile / params2 feed	TAPE6.OUT TAPE7_$.TEM = TAPE7_$.OUT
17	Modify previous MCNP input file by adding new compositions, and tally isotopes if deemed "important" (monteb 7m)	TAPE7_$.OUT TAPE9_$.INP mbxs.inp mcnp_$.inp mnat_$.tmp	mb4_$.out mb7_$.out mat_$.inp tmpfile / T9err_$.TXT mbmc.skl
18	Create full MCNP input file from user-generated version, including tallies (monteb 3)	mbmc.skl mat_$.inp tal1-3_$.inp	mbmc(.dat)

TABLE 1 (cont)
PROCEDURE

Step	Process	Input[a]	Output[a]
19	Run MCNP to calculate one-group cross-sections and fluxes	mbmc(.dat)	mbmco(.dat)
20	Modify ORIGEN2 file with new cross-section and flux values obtained by MCNP (monteb 6m)	feed mbmco TAPE7_$.OUT TAPE9_$.INP tmpfile/TAPE5_$.# tmpfile/params2	mb1-3,6,8,14-17_$.out mb11.out tmpfile/mtu_$.tmp TAPE9_$.INP tmpfile/TAPE5_$.t#
21	Run ORIGEN2 for entire step. Print results halfway to compare with predictor step(s) and then perform discrete removal (includes monteb 8e and two ORIGEN2 runs)	tmpfile/TAPE5_$.# = TAPE5_$.INP TAPE4_$.INP TAPE9_$.INP tmpfile/params2 feed mbmco(.dat)	TAPE6.OUT TAPE7_$.TEM = TAPE7_$.OUT mb14-17_$.out mb5.._$.out
22	Save information for a restart case	TAPE9_$.INP TAPE7_$.OUT mbmc(.dat) mb.inp	tmpfile/TAPE9_$.# tmpfile/TAPE7_$.# tmpfile/mbmc.# tmpfile/mbinp.#
23	Modify previous MCNP input file by adding new compositions of materials (monteb 7e)	TAPE7_$.OUT TAPE9_$.INP mbxs.inp mcnp_$.inp mnat_$.tmp	mb7_$.out mat_$.inp tmpfile/T9err_$.TXT
24	Run MCNP for complete outer step	mbmc.skl mat_$.inp	mbmco(.dat)
25	Obtain criticality values from MCNP output file (monteb 6e)	mbmco(.dat) tmpfile/params2 feed	mb11_$.out
26	Remove discrete removal group elements (monteb d)	tmpfile/params2 feed TAPE7_$.OUT	tmpfile/TAPE7_$.O#
27	Output results of ORIGEN2 (monteb 8e)	mbmco(.dat) TAPE7_$.OUT TAPE9_$.INP	mb14-17_$.out mb5.._$.out

TABLE 1 (cont)
PROCEDURE

Step	Process	Input[a]	Output[a]
28	Calculate the amount of material burned and produced based on feed and inventory information (monteb z)	mb5t_$.out mb5tx_$.out mb12a_$.out mb9t_$.out tmpfile/params2	mb9_$.out mb9t_$.out mb10.txt mb10t_$.out
29	Reduce resulting number of input files to two	mb@t_$.out mb@.txt	***.chk ***.out

TABLE 2
SUMMARY OF FILES USED IN *MONTEBURNS*

File	Description [a,b]
******* mbmc mbmc.skl /tmpfile/mbmc.#	MCNP input file created by user (user can choose any name *** that meets MCNP requirements: i.e., no more than 7 characters) Name of MCNP input file used by *monteburns* (initially = ***) Skeleton MCNP input file (based on ***) Name of MCNP input files saved for restart runs (# = outer burn step)
mat_$.inp	Contains modified MCNP material cards after each burn step
tal1_$.inp tal2_$.inp tal3_$.inp	These three files contain commands that are used to generate the flux spectrum, cross-section, and other tallies in MCNP. These files are merged with the MCNP input file before MCNP is run (except for intermediate criticality only runs).
mbxs.inp	This file lists the default MCNP cross-section library to be used for each isotope if is not already identified.
mbmco mbmcr mbmcs	Default name of MCNP output files
*****.feed** feed	Optional input file created by user, contains feed/removal and time-step information Name of default feed file used in *monteburns* (initially = ***.feed)
*****.inp** mb.inp tmpfile/mbinp.#	Input file created by user, contains code specific variables Name of default input file used in *monteburns* (initially = ***.inp) Name of input files saved for restart runs
TAPE9_$.INP TAPE9_$.TMP TAPE9_0.INP tmpfile/TAPE9_$.I#	Contains values from the ORIGEN2 decay and cross-section libraries. This file goes through various temporary stages, which include replacing ORIGEN2 cross-section values with ones obtained from MCNP. The variations listed to the left represent the temporary files, the last of which is used for restart runs

[a]The bolded file names represent those supplied by the user.
[b]The following symbols apply for the table: # = number of current outer burn step, $ = number of current material being analyzed, *** = base name of files.

TABLE 2 (cont)
SUMMARY OF FILES USED IN *MONTEBURNS*

File	Description [a, b]
tmpfile/T9err_$	Displays errors incurred from finding cross-section values in fort_$.9
TAPE4_$.INP TAPE7_$.OUT TAPE7_$.TMP TAPE7_$.TEM tmpfile/TAPE7_$.O#	Contains the names of isotopes and their number densities that will be processed in ORIGEN2, units are in gram-atoms (fort.4 = ORIGEN2 input, fort.7 = ORIGEN2 output, # = outer burn step)
orig21/Decay.lib orig##/^^^.lib	'orig21' is the identifier of the ORIGEN2 decay library ## then identifies the cross-section library requested by the user or ^^^ is the name
mcnp_$.inp	Contains a list of isotopes/elements in the initial MCNP input file
mnat_$.tmp	Contains a list of natural elements from the initial MCNP input file
TAPE5_$.INP TAPE5_$.TMP /tmpfile/TAPE5_$.#I	Working ORIGEN2 input file Temporary ORIGEN2 input files (# = outer burn step)
TAPE6.OUT	Working ORIGEN2 output file
tmpfile/params tmpfile/params2 tmpfile/para3_$ tmpfile/param_$.# tape.tmp	Temporary files used by *monteburns* to read input parameters and to determine if discrete feed exists or not for each outer burn step (#). ***Below:*** **Individual output files from *monteburns***
mb1.txt&mb1t_$.out, mb2.txt&mb2t_$.out, mb3.txt&mb3t_$.out, mb4a.txt&mb4a_$.out, mb4b.txt&mb4b_$.out, mb5.txt,mb5t_$.out, mb5x_$.out &mb5tx_$.out mb6.txt&mb6t_$.out, mb7.txt&mb7t_$.out, mb8.txt&mb8t_$.out, mb9.txt&mb9t_$.out, mb10.txt&mb10_$.outmb 11t_$.out mb12.txt&mb12t_$.out mb12x&mb12tx_$.out mb13t_$.out mb14.txt,mb14t_$.out mb15.txt,mb15t_$.out mb16.txt,mb16t_$.out mb17.txt,mb17t_$.out	mcnp results: k_{eff}, nu,flux, variance, and cross-sections n,gamma for automatic and important isotopes n,fission for tracked isotopes spectrum for predictor steps inventory of tracked isotopes at halfstep (predicted) inventory of tracked isotopes at halfstep (actual) inventory of tracked isotopes at halfstep (with precision for more calc) flux spectrum during steps materials sent back to mcnp each time it is run fission-to-capture ratio feed and burnup of tracked isotopes, total actinide, and final summary feed and burnup rates mcnp results: day (time of cumulative irradiation), k_{eff}, and variance inventory of materials at the beginning of each step beginning inventory (with greater precision) k_{eff} at beginning of each step activity of tracked isotopes at end of step (Ci) heatload of tracked isotopes at end of step (W) inhalation toxicity of isotopes at end of step (m^3 air) ingestion toxicity of isotopes at end of step (m^3 water)
***.chk, ***.out	Final output files from *monteburns*

3.3. ORIGEN2 Description

ORIGEN2 performs burnup calculations for *monteburns* using the matrix exponential method.[2] ORIGEN2 considers time-dependent formulation, destruction, and decay concurrently.[3] These calculations require (1) the initial compositions and amounts of material, (2) one-group microscopic cross-sections for each isotope, (3) material feed and removal rates (if desired), (4) the length of the irradiation period(s), and (5) the flux or power of the irradiation. The user must give this information in the input files discussed in Section 5.0.

Input files for ORIGEN2 are complicated to write, and output files generated by ORIGEN2 are bulky and complicated to read. Thus, *monteburns* eliminates the user's need to create his/her own ORIGEN2 input files and to extract information from ORIGEN2 output files. *Monteburns* provides a "cross-section and decay information" file, *TAPE9.INP*; a file with material compositions, *TAPE4.INP*; and a skeleton ORIGEN2 file, *TAPE5.INP*, which contains commands and continuous feed and removal information.

3.4. Calculations

A number of calculations are performed by *monteburns*. They are divided into six different categories and are presented below. These categories are (1) energy per fission, (2) flux normalization, (3) reactor physics constants, (4) effective multiplication factor, (5) power, and (6) fractional importance.

3.4.1. Energy per Fission

The user has two options of how to calculate the amount of energy deposited per fission for a system. First, he/she can enter the desired Q-value (the average for the entire system) into the *monteburns* input file. Second, the user can enter a Q-value for ^{235}U that he/she thinks is most representative of the nuclear system being evaluated (preceded by a negative sign in the input file. The code will calculate the average Q. In this case, the following equations are used by *monteburns* to calculate the amount of energy per fission for each material [see Eq. (4) for the Q-value for the entire system] according to the distribution of various actinides in the material.

The value of Q entered must include all modes of energy deposition, including fission gammas, capture gammas, and neutron kinetic energy. It would be more accurate to run MCNP in the "nps" mode and tally energy deposition, but this would require considerably more computation time. The current method should be sufficiently accurate except in cases where (n,γ) heating varies significantly as the isotopes of the system change. Future code modifications may address this issue.

$$Q_{fis} = \left|Q_{U-235}\right| * Q_{rat} \quad , \tag{1}$$

where

Q_{fis} =total amount of recoverable energy produced per fission,

Q^{235}_{U-} =recoverable energy per fission for ^{235}U [input by user—recommended value is 200 MeV (Ref 4)], and

Q_{rat} =weighting factor to include recoverable fission energy for all actinides present;

$$= \sum_{i=1}^{n} q_{rat}(i) * f_{rat}(i) \quad , \tag{2}$$

where

n =number of isotopes being considered,

$q_{rat}(i)$ = ratio of recoverable energy per fission for isotope i divided by the recoverable energy per fission for ^{235}U (Ref 5) and listed in Table 3, and

$f_{rat}(i)$ =ratio of fissions resulting from isotope i to total number of fissions [see Eq. (3)];

$$= \frac{\sigma_f(i) * n(i)}{\sum_{i=1}^{n} (\sigma_f(i) * n(i))} \quad , \tag{3}$$

where

$\sigma_f(i)$ = one-group microscopic fission cross-section of isotope, and

$n(i)$ = number density of isotope i in the system (in units of gram-atoms).

TABLE 3
FRACTION OF RECOVERABLE ENERGY PER FISSION FOR CERTAIN ACTINIDES DIVIDED BY THE RECOVERABLE ENERGY PER FISSION FOR ^{235}U

Isotope	Fraction	Isotope	Fraction
^{227}Th	0.9043	^{240}Pu	1.0379
^{229}Th	0.9247	^{241}Pu	1.0536
^{232}Th	0.9573	^{242}Pu	1.0583
^{231}Pa	0.9471	^{241}Am	1.0513
^{233}Pa	0.9850	^{242m}Am	1.0609
^{232}U	0.9553	^{243}Am	1.0685
^{233}U	0.9881	^{242}Cm	1.0583
^{234}U	0.9774	^{243}Cm	1.0685
^{235}U	1.0000	^{244}Cm	1.0787
^{236}U	0.9973	^{245}Cm	1.0889
^{237}U	1.0074	^{246}Cm	1.0991
^{238}U	1.0175	^{248}Cm	1.1195
^{237}Np	1.0073	^{249}Cm	1.1296
^{238}Np	1.0175	^{251}Cf	1.1501
^{238}Pu	1.0175	^{254}Es	1.1807
^{239}Pu	1.0435		

Next, the average energy deposited per fission in the system as a whole can be calculated.

$$Q_{ave} = \frac{\sum_{j=1}^{m} (Q^j_{fis} * \phi^j_n * \Sigma^j_f * V^j)}{\sum_{j=1}^{m} (\phi^j_n * \Sigma^j_f * V^j)} \quad , \tag{4}$$

where

Q_{ave} = the average recoverable energy per fission for all materials,
Q^j_{fis} = average energy per fission for material j (MeV),
ϕ^j_n = value of flux of material j obtained from MCNP output file,
Σ^j_f = macroscopic fission cross-section of material j (cm^{-1}),
V^j = total volume of all cells containing material j (cm^3), and
M = number of materials being analyzed

3.4.2. Flux Tally Normalization/Reactor Physics Constants

For each material j, the value of the flux that is used for burnup calculations in ORIGEN2 is calculated from the flux tallied by MCNP (which is normalized per MCNP source neutron):

$$\phi = \phi_n * C \quad , \tag{5}$$

where

ϕ = true value of the flux (normalized to system power), and
C = a constant [see Eqs. (7) or (9)].

When an MCNP input file with a "kcode" (criticality) source definition is used and k_{eff} and its associated error are found from the MCNP output file, then the value of C is as follows:

$$C = \frac{\upsilon * P * 10^6 \, W/MW}{(1.602 \times 10^{-13} \, J/MeV) * k_{eff} * Q_{ave}} \quad , \tag{6}$$

where

υ = average number of neutrons produced per fission (see the next section for calculation of υ),

P = power defined by user for each material (in MW), and

k_{eff} = effective multiplication factor obtained by MCNP.

When the MCNP input is a "sdef" source definition, then the value of C is instead

$$C = \frac{src * P * 10^6 \, W/MW}{floss * (1.602 \times 10^{-13} \, J/MeV) * Q_{ave}} \quad , \tag{7}$$

where

src = weight of source neutrons (approximately equal to one), and
floss= weight of neutrons lost to fission.

3.4.3. Reactor Physics Constants

For both types of source definitions, the value of υ can be calculated from results in the MCNP output file. For a "kcode" source definition, υ is calculated as follows:

$$\upsilon = k_{eff} * src/floss \quad , \tag{8}$$

where

src = weight of source neutrons (approximately equal to one), and
floss= weight of neutrons lost to fission.

For a "sdef" source definition, the value of υ is

$$\upsilon = fsrc / floss \ , \tag{9}$$

where

fsrc = weight of source neutrons gained in fission.

For either type of MCNP input file, the number of neutrons produced per neutron destroyed (η) is

$$\eta = \frac{(\upsilon\sigma_f + 2.0 * \sigma_{n2n} + 3.0 * \sigma_{n3n})}{(\sigma_a + \sigma_f)} \ , \tag{10}$$

where

σ_f = fission cross-section from MCNP,
σ_γ = (n,γ) cross-section from MCNP,
σ_{n2n} = (n,2n) cross-section from MCNP,
σ_{n3n} = (n,3n) cross-section from MCNP, and
σ_a = total absorption cross-section from MCNP (-2 reaction tally type).

3.4.4. Effective Multiplication Factor

The value of the effective multiplication factor for an "sdef" source definition must be calculated from the value of the net multiplication obtained from the MCNP output file:

$$k_{eff} = \frac{(fmult - 1)}{(fmult - 1/\upsilon)} \ , \tag{11}$$

where

fmult = net multiplication in the system.

The relative error (σ) associated with k_{eff} is then

$$\sigma = \frac{\{(fmult*(1+err) - 1) - k_{eff}\} / k_{eff}}{(fmult*(1+err) - 1/\upsilon)} \quad , \tag{12}$$

where

err = relative error associated with the net multiplication in the system.

3.4.5. Power

Finally, the power produced by each material is

$$P^j = \frac{(Q_{ave} * \phi^j * \Sigma_f^j * V^j * 1.60219*10^{-13} J/MeV)}{10^6 W/MW} \quad , \tag{13}$$

where

P^j = power produced by material j (MW), and
ϕ^j = flux of neutrons in material j ($n/cm^2/sec$).

3.4.6. Fractional Importance

The fractional importance calculations help determine which isotopes are considered "important" to the overall burnup calculation and which are not. If any of the following values (atom fraction, weight fraction, fraction of absorption, and fraction of fission) are greater than the value of the "fractional importance" assigned by the user, then the isotope is considered "important" and is included in all transfers from ORIGEN2 to MCNP and back throughout the remainder of the run (see Section 4.2 for more information).

$$a_{fi} = \frac{gad_i}{\sum_{i=1}^{n} gad_i} \quad , \tag{14}$$

$$w_{fi} = \frac{gad_i * A_i}{\sum_{i=1}^{n} (gad_i * A_i)} \quad , \tag{15}$$

$$f(\sigma_a)_i = \frac{gad_i * \sigma_{ai}}{\sum_{i=1}^{n} (gad_i * \sigma_{ai})} \quad , \tag{16}$$

and

$$f(\sigma_f)_i = \frac{gad_i * \sigma_f}{\sum_{i=1}^{n} (gad_i * \sigma_f)} \quad , \tag{17}$$

where

i = isotope being studied,
n = total number of isotopes in system,
a_{fi} = atom fraction of isotope i in system,
w_{fi} = weight fraction of isotope i in system,
$f(\sigma_a)_i$ = fraction of absorption isotope i contributes to system,
$f(\sigma_f)_i$ = fraction of fission isotope i contributes to system,
gad_i = amount of isotope in system in gram-atoms,
A_i = atomic weight of isotope i in grams,
σ_{ai} = microscopic absorption cross-section of isotope i, and
σ_{fi} = microscopic fission cross-section of isotope i.

3.4.7. Activity, Heatload, and Radiotoxicities

When studying radioactive waste and waste repositories (as well as other applications), it is important to keep track of many things beyond the grams of material at the beginning and end of each burnup step. In fact, some of the most important quantities to calculate are the activity of isotopes in each material as a function of burnup (activation in Curies), the heatload (decay power in Watts), and inhalation and ingestion radiotoxicities (m^3 in air and water, respectively).

The following equations are used in *monteburns* to calculate activity, heatload, inhalation, and ingestion toxicities respectively.

$$Act = m * SA \tag{18}$$

and

$$SA = \frac{\ln(2) * N_a}{A * T_{1/2} / 3.7 * 10^{10} Bq/Ci} \quad , \tag{19}$$

where

Act = activity of isotope in Ci,

SA = specific activity (Ci / g [activity per gram of material (Ref. 7)],

m = mass of nuclide (g / mole),

N_a = Avogadro's number = $6.022*10^{23}$ atoms / mole,

A = atomic weight of nuclide (g),

$T_{1/2}$ = half-life of nuclide (s), and

Bq = disintegrations / s (assume one atom / disintegration).

$$HL = Act*3.7*10^{10}\,Bq/Ci*Q_{rec}*10^{6}\,eV/MeV*1.6012*10^{-19}\,J/eV \quad (20)$$

where

HL = heatload (decay power) released by isotope (W), and

Q_{rec} = average recoverable energy emitted from decay events (MeV), (values obtained from ORIGEN2 decay library).

$$InhTox = \frac{\ln 2 * N}{T_{1/2} * C_{inh}} \quad (21)$$

and

$$IngTox = \frac{\ln 2 * N}{T_{1/2} * C_{ing}} \quad , \quad (22)$$

where

$InhTox$ = inhalation toxicity of nuclide (m^3 air),
$IngTox$ = ingestion toxicity of nuclide (m^3 water),
N = number of atoms of nuclide, and
C = radioactivity concentration limit (Ref. 6).

4.0. USER INTERACTIONS WITH THE SOFTWARE

The primary role of the user in this program is to create the required two to four input files. A description of input parameters is presented below, and the format of the input files is shown in Section 5.0.

4.1. Required Input Files

The user must generate two to four different input files before executing *monteburns*. The two required input files are the MCNP input file (designated here by *mbfile,* but can be any name up to 8 characters), and a general *monteburns* input file (this must have the same prefix "mbfile" with an extension of ".inp" for a name of *mbfile.inp*). For many complex burnup scenarios, the user must also generate a feed input file (with a name of *mbfile.feed*), which contains detailed instructions for *monteburns* at each time step (i.e., time interval, power, and material feed/removal). The only case in which a feed input file is not required is for a constant power burn with no material feed or removal. Finally, *monteburns* uses one other input file, *mbxs.inp,* which contains a list of default MCNP cross-section identifiers for isotopes that may be produced in the irradiation process and are not initially specified by the user. A sample of this file is included with the *monteburns* source code package; this sample file can be modified as requirements dictate (see Section 5.4 for more information).

4.2. Main Input Parameters

The user is required to know many input variables to run this code. The parameters are described below; Section 5.0 discusses how each of these parameters is entered into input files.

- **Number of MCNP materials**—this indicates the number of materials the user wants to irradiate from the MCNP input file (i.e., transfer back and forth between MCNP and ORIGEN2). Note: The current limit on the number of materials is 49.

- **MCNP material number(s)**—the identification number of the material(s) in the MCNP input file for which a burnup analysis is desired (*monteburns* will tally average results over all cells and parts of a repeated structure or lattice that contain this material). If a user desires to obtain information for a material (i.e., flux, cross-sections, etc.) without burning the material in ORIGEN2, then he/she can enter the number of that material here preceded by a negative sign to indicate that it will not be irradiated (however, that material will still be decayed in ORIGEN2). Note: the number of entries here must equal the number of MCNP materials entered above. Additionally, the order in which these material numbers are listed define what *monteburns* material number is assigned to each MCNP material number (this will be used for determining what material is in each region—see Section 5.3 for more information). For example, if MCNP material 1 is listed first followed by 5 and 10, then *monteburns* material 1 is initially defined to be MCNP material 1, *monteburns* material number 2 is MCNP material 5, and *monteburns* material number 3 is initially comprised of MCNP material 10.

- **Material volume(s)**—the sum of the volume (cm^3) of all cells in the MCNP input file for each material number(s) listed above (again, the number of entries must equal the number of MCNP materials). If the user enters a value of 0.0 for one or more of these, then the volume calculated by MCNP is used (if it exists). However, often the geometry is too complex for MCNP to calculate the volume. In this case, unless the user has input a non-zero volume for that material number, an error message appears, *monteburns* terminates, and it must be rerun with non-zero values. Additionally, in most cases of repeated structures, MCNP calculates the volume of cells containing a given material incorrectly. For each of these cases (and for any other instances the user desires), the user must enter the sum of the volumes of cells containing each material being analyzed.

- **Total power of the system**—the power (MW) generated by the entire system represented in the MCNP model (this is not necessarily the same as the power generated solely by the materials burned in *monteburns*). This value, along with the recoverable energy per fission, is used to normalize the flux from MCNP in each burned region for ORIGEN2. Additionally, the user can enter the fraction of this power to be used during each outer burn step (if power is not constant over the entire burn) in the feed input file. By entering a power fraction of zero for a step, it effectively becomes a decay-only step, which is useful for analyzing cooling periods of systems. Note: the value of fission power output is subject to statistical errors and may not be exactly the same as the power input. Increased statistics in MCNP may minimize this problem; nonetheless, the user should check the value of power output to ensure that it is close to the amount of power initially desired.

- **Recoverable energy per fission**—this value represents the average recoverable energy per fission (Q) in MeV in the aforementioned MCNP model. If the user does not know the exact amount of energy generated by a combination of several isotopes, then he/she can enter the recoverable energy per fission for ^{235}U for that system (commonly ~200 MeV for light-water reactors), preceded by a negative sign. The negative sign means that the value of the recoverable energy per fission will be calculated by *monteburns* based on the fissile isotopics of the system. In this case, Q is calculated as the sum of all actinide Q fractions, which are based on the fraction of fissions caused by a specific isotope times the Q of that isotope divided by the Q of ^{235}U (see Eqs. 1–4 for more information). WARNING: the fissile isotopics used for the calculation of Q are based only on the materials burned by *monteburns*. If the fissile isotopics of the entire system are significantly different from the fissile isotopics of the materials being burned, then the average value of Q may be in error. Thus, the flux normalization may be in error (although in most cases, this should be a relatively small effect).

- **Total number of days burned**—this number represents the length of time for which a material is irradiated in ORIGEN2 (or the decay time if the power equals zero). If the user provides a feed input file, then the irradiation lengths (in days) for each outer burn step (described below) must be provided in this file and a value of 0.0 entered in the *monteburns* input file. Otherwise, the total irradiation time (in days) must be entered in the *monteburns* input file.

- **Number of outer burn steps**—this number indicates how many outer burn steps are desired. If a feed input file exists, this must equal the number of steps described in the feed input file. If a feed input file does not exist, the length of the irradiation period for each outer burn step equals the total days burned divided by the number of outer burn steps. Each of these steps represents a time period for which a burnup calculation is performed, and representative cross-sections are obtained (the burn step then uses spectrum-averaged, one-group, cross-sections calculated at a predictor step halfway through that step). Each outer step can also indicate the addition and/or removal of a material.

- **Number of internal burn steps**—this is the number of additional times into which the irradiation period is divided for ORIGEN2 calculations. As mentioned in Section 3.0, the results obtained from ORIGEN2 (and as a result, *monteburns*) may be more accurate if long irradiation periods are broken up into smaller lengths of time, especially at the beginning of a system's life. This is because the Bateman equations are used instead of the Gauss-Seidel iterative technique to solve for compositions of materials when the half-life of an isotope is <10% of the irradiation interval. Therefore, results may vary according to which technique is used.[8] Additionally, the physics and composition of materials in the system may change significantly with time. Thus, the user can specify that the outer burn steps be divided into even smaller time segments for use in ORIGEN2. In addition, there is virtually no penalty on execution time by using smaller time steps in ORIGEN2 because most of the execution time lies with MCNP.

- **Number of predictor steps**—this is another variable affecting the accuracy of the results. As the isotopic composition of a material changes during an irradiation step (both due to burnup and potential variances in continuous feed from beginning to end), the cross-sections may change as well. To obtain the most accurate results, spectrum-averaged, one-group cross-sections for a burn step should represent an average over the time interval. In a *monteburns* calculation, ORIGEN2 is run halfway through each outer burn step, and the resulting isotopics are used in MCNP to calculate spectrum-averaged, one-group cross-sections and fluxes for that

step. Then a complete ORIGEN2 run is performed with the new values to determine final compositions. This assumes that the isotopics of the system at the midpoint are a reasonable approximation of the isotopics over the entire burn step, and that cross-sections are representative of the step (actually it is only important that the neutron flux energy spectrum be representative of the entire burn step). The user must be aware of this assumption and consequently ensure that burn intervals are not too long.

If the initial cross-sections for a step are not accurate, then the ORIGEN2 compositions halfway through the step may not be a good representation of the burn step. Thus, it is often beneficial to perform a "predictor" step (derived from a basic form of the predictor-corrector method) to calculate cross-sections more than once at the midpoint of a burn step and to compare the neutron energy spectrum and isotopic compositions halfway through the step (these values are printed in the output files) to make sure that the final cross-sections are representative of the system at that step. The number of times for which cross-sections are calculated halfway through each step is the number of predictor steps. Executing multiple predictor steps increases the accuracy of the burnup calculation because the spectrum-averaged, one-group cross-sections used to perform the predictor step approach the ones calculated by the predictor step (i.e., they converge). In addition, *monteburns* automatically adds a predictor step for the initial burn step because the actual spectrum-averaged, one-group cross-sections for a system may be different than those supplied in the chosen default ORIGEN2 library. This problem can be partially avoided by providing an initial library that has been previously generated by *monteburns* for a similar system instead of using one of the ORIGEN2 default libraries (see the "Identifier for ORIGEN2 library" bullet below for more information). For all subsequent burn steps, *monteburns* uses the modified spectrum-averaged, one-group cross-section library from the previous burn step; thus, an extra predictor step is not required.

- **Step to restart after**—a user can use this parameter to restart a run that ends unexpectedly or to branch off from a previous *monteburns* run with different input variables (for example, if k_{eff} drops too low during the n^{th} burn step, the user can change the feed rate for the n^{th} step and restart from the previous step). The "restart step" indicates the outer burn step after which *monteburns* should start, using all previously created input files and results for the outer burn steps up to that point. To use this variable effectively, all input files that were created by *monteburns* during the previous run must remain in the *tmpfile* subdirectory of the directory in which *monteburns* previously ran. If a restart run is not being performed, then the "restart step" value should be zero. This value gets modified during each step to reflect the value of the current step. *Monteburns* appends data obtained from the restart run to the existing output files so that easier comparisons can be made. As a result, some of the

production / destruction data may not be accurate, and an "Abort" error will occur because it cannot be read correctly. This has no impact on the other results and should be ignored.

- **Identifier for ORIGEN2 library**—this identifies from which ORIGEN2 library initial cross-section values are obtained (they are modified to be system-dependent after the first step). The ORIGEN2 manual[8] contains a list of over 30 different cross-section libraries for different types of systems from which the user can choose. Each of these libraries should have been provided with the source code from Radiation Safety Information Computational Center (RSICC) and is associated with either an *orig##* file, where ## is a number used to identify the library or a "*name.lib*" (or "*NAME.LIB*" in VMS), where "name" and "##" are identified in Table 4. Either the value of this two-digit number or the associated name (WITHOUT the *.lib* extension) must be entered by the user. If the user generates his / her own ORIGEN2 library (i.e., from a previous *monteburns* run) to be used as the initial library, he / she must give it a name (orig## or "*name*") that does not currently exist and place it in the proper library location (see below) and must reference it within the FORTRAN77 program (see the authors for more guidance about doing this).

- **ORIGEN2 library location**—this line of input must contain the location of the ORIGEN2 libraries (both decay and cross-section) in the user's file space or in the directory of another user on the system that has the library files. This way, only one user on a UNIX operating system needs to have a copy of the libraries. The decay library must also appear in this location as orig21 (for the "##" input above) or Decay.lib / DECAY.LIB, along with the appropriate cross-section library(ies).

- **Importance fraction**—this value represents the lower limit (tolerance) for the importance of one isotope relative to the rest of the system based on results obtained from ORIGEN2 and MCNP. If an isotope contributes a large enough fraction (i.e., greater than the importance fraction) to absorption or fission interactions, mass, or atom density (see Section 3.2.6 for more information), then the isotope is considered "important." Flux and one-group, spectrum-averaged, cross-section tallies are then performed in MCNP for this isotope. If the importance fraction is zero, then all activation, fission products, and actinides generated in ORIGEN2 are tallied (except those for which no MCNP cross-section exists—see Section 3.3.4 for more information). If the importance fraction is one, then no isotopes are deemed "important" except those specified as "automatic" in the input. Additionally, it is advised that the initial ORIGEN2 library is somewhat representative of the system, or "important" isotopes may not be properly identified. The only way to absolutely avoid this problem is to track every isotope or to generate a problem-specific library with a

TABLE 4
INITIAL CROSS-SECTION LIBRARIES PROVIDED BY ORIGEN2

Library	Character Identifier (VMS)	Number Identifier (UNIX)
PWR: ^{235}U-enriched UO_2 with a burnup of 33,000 MWd/MTU	PWRU	orig22
PWR: ^{235}U-enriched UO_2 in a self-generated Pu recycle reactor	PWRPUU	orig23
PWR: Pu-enriched UO_2 in a self-generated Pu recycle reactor	PWRPUPU	orig24
PWR: ThO_2-enriched with denatured ^{233}U	PWRDU3TH	orig25
PWR: ThO_2-enriched with recycled, denatured ^{233}U	PWRD5D33	orig26
PWR: ThO_2-enriched with makeup, denatured ^{235}U	PWRD5D35	orig27
PWR: Pu-enriched ThO_2	PWRPUTH	orig28
PWR: ^{235}U-enriched UO_2 with a burnup of 50,000 MWd/MTU	PWRU50	orig29
BWR: ^{235}U-enriched UO_2	BWRU	orig30
BWR: ^{235}U-enriched fuel in a self-generated Pu recycle reactor	BWRPUU	orig31
BWR: Pu-enriched fuel in a self-generated Pu recycle reactor	BWRPUPU	orig32
Thermal: 0.0253 eV cross-sections	THERMAL	orig33
CANDU: Natural	CANDUNAU	orig34
CANDU: Slightly Enriched	CANDUSEU	orig35
LMFBR: Advanced Oxide, LWR-Pu/U/U/U Core	AMOPUUUC	orig36
Axial Blanket	AMOPUUUA	orig37
Radial Blanket	AMOPUUUR	orig38
LMFBR: Early Oxide, LWR-Pu/U/U/U Core	EMOPUUUC	orig39
Axial Blanket	EMOPUUUA	orig40
Radial Blanket	EMOPUUUR	orig41
LMFBR: Advanced Oxide, recycle-Pu/U/U/U Core	AMORUUUC	orig42
Axial Blanket	AMORUUUA	orig43
Radial Blanket	AMORUUUR	orig44
LMFBR: Advanced Oxide, LWR-Pu/U/U/Th Core	AMOPUUTC	orig45
Axial Blanket	AMOPUUTA	orig46
Radial Blanket	AMOPUUTR	orig47
LMFBR: Advanced Oxide, LWR-Pu/Th/Th/Th Core	AMOPTTTC	orig48
Axial Blanket	AMOPTTTA	orig49
Radial Blanket	AMOPTTTR	orig50
LMFBR: Advanced Oxide, 14% denatured ^{233}U/Th/Th/Th Core	AMO1TTTC	orig51
Axial Blanket	AMO1TTTA	orig52
Radial Blanket	AMO1TTTR	orig53
LMFBR: Advanced Oxide, 44% denatured ^{233}U/Th/Th/Th Core	AMO2TTTC	orig54
Axial Blanket	AMO2TTTA	orig55
Radial Blanket	AMO2TTTR	orig56
LMFBR: Advanced Oxide, recycle-^{233}U/Th/Th/Th Core	AMODTTTC	orig57
Axial Blanket	AMODTTTA	orig58
Radial Blanket	AMODTTTR	orig59
LMFBR: FFTF Pu/U	FFTFC	orig60
ATW (created by TSA-10 at LANL)	ATW	orig65

previous run of *monteburns* that replaces the original default ORIGEN2 library (see the "Identifier for ORIGEN2 library" bullet above for more information).

The user must also decide how to deal with fission products. If the user enters the importance fraction as a positive value, then only those fission products deemed "important" are included in MCNP. However, because MCNP cross-sections for many fission products do not exist, *monteburns* contains the option to lump all fission products together as one sum (except for those fission products, if any, designated as "automatic" in the *monteburns* input file) by using a negative value here. These lumped fission products are then given one of two general fission product cross-sections in MCNP—the average fission product from ^{235}U and the average fission product from ^{239}Pu (these have the identifiers 45117 and 46119 respectively[1]). The fraction of the total fission product mass separated into each category is determined by comparing the number of fissions that result from isotopes with an atomic number less than or equal to that of uranium (92) to those that occur in other transuranic actinides with an atomic number >92. Note: the use of this attribute has not been fully benchmarked or documented, and the 45117 and 46119 data may be inaccurate for many applications, so exercise caution when using it! However, by developing representative cross-sections for such fission products and naming them 45117 and/or 46119 (with extensions other than the MCNP ones of .90c and .90d), the user can have more control over the data and know exactly where it came from.

- **Intermediate flag**—this flag indicates whether or not intermediate k_{eff} calculations are performed. Normally, MCNP is only run once per predictor step, and these runs occur half way through each outer burn step (i.e., half way through each irradiation period). However, it is often desired to obtain a value of k_{eff} at the beginning and/or end of each burn step. When the value of this parameter is one, additional MCNP calculations are performed to determine k_{eff}. Neither cross-sections nor fluxes are recalculated by MCNP for these runs, so ORIGEN2 results are not influenced. The only purpose of the "intermediate" MCNP calculations is to provide the value of k_{eff} at more than one point during each outer burn step to see how the system changes. When a discrete feed addition (see Section 3.3.3) occurs, three MCNP runs are performed for the step (at the beginning, middle, and end); otherwise, two MCNP runs are performed (at the middle and end) because the beginning value of k_{eff} equals the ending value of k_{eff} from the previous step. If the value of this parameter is zero, then only one MCNP run is performed for each outer burn step (in the middle) regardless of whether or not the discrete feed occurs.

- **Number and list of automatic tally isotopes for each material**—this integer represents the number of isotopes/elements for which the user wants tallies to be performed in MCNP and results written to *monteburns* output files (i.e., automatic "important" isotopes). The user must then enter the MCNP identification number for each of these isotopes/elements (these can indicate library preference and/or temperature dependence). It also allows the user to use a cross-section not specified in the default cross-section file discussed in Section 5.4, *mbxs.inp* (i.e., the cross-section identifier listed here has precedence over the one in *mbxs.inp*). The current limit on the total sum of the isotopes in all materials combined is slightly above 9000.

4.3. Feed Input Parameters

The purpose of a feed input file in *monteburns* is to list the lengths of each time step, to vary the fraction of power generated by the system during each time step, to shuffle materials from one region to another, and/or to specify amounts of materials to add to or remove from the system during each outer burn step. The user can also specify continuous or discrete (all at one time) feed (addition of isotopes) and/or removal (of specified elements) for each material at each time step in this file. First, for each outer burn step and material (for most items), the user enters the following parameters:

- length of the irradiation (in days)
- fraction of power produced relative to the total power entered in the *monteburns* input file
- region in which each material is located
- feed group (defined below)
- feed rate(s) (both beginning and ending rates for continuous and a flag and a rate for discrete)
- removal group numbers (positive for continuous feed, negative for discrete
- removal fraction [the fraction of each element removed (e.g., a fractional removal of 0.9 means that 90% of the removal group is removed and 10% remains)].

5.0. DESCRIPTION OF INPUT FILES

This section describes the four input files that *monteburns* uses, including (1) the MCNP input file, (2) the *monteburns* input file, (3) the feed input file, and (4) a cross-section map.

5.1. MCNP Input File

To execute *monteburns*, the user must have enough knowledge of MCNP to create an MCNP input file for the system that he/she wishes to analyze using either the "kcode" or "sdef" source definition. There is no required format of this input file in *monteburns*, except that material and user tally numbers must not be >100 (this is to keep *monteburns* tallies from interfering with user input), and it must be executable in MCNP. Note: This means it must also have at least 30 active kcode cycles to produce enough results to be analyzed by MCNP and thus *monteburns*. Explicit use of source files (*srctp*) is not yet supported; the source must be defined in the MCNP input file. A simple MCNP input file is included as Appendix A, and a more complex one (that will include a multimaterial burn) is in Appendix C.

5.2. *Monteburns* Input File

Another file that the user must create is an input file describing parameters required for the operation of *monteburns*. These parameters were described in detail in Section 4.2 and are listed along with appropriate format specifications in Table 5. A corresponding, simple (no feed or intermediate k_{eff} calculations) *monteburns* input file to go with the MCNP input file in Appendix A is displayed in Appendix B; one corresponding to Appendix C is in Appendix D.

5.3. Feed Input File

The feed input file allows the user to add or remove different amounts of materials to the system during each outer burn step, vary the power produced during each time interval for an irradiation, and/or shuffle materials from one region to another. The format of a feed input file is free, so the user can enter as large of numbers for each variable as desired as long as there are spaces in between variables.

TABLE 5
DESCRIPTION OF *MONTEBURNS* INPUT FILE

Parameter	Format	Description	Example
72-character title	72-char.	Briefly identifies scenario.	ATW system w/Tc99
Operating System	4-char	What operating system user is on: UNSU = UNIX Sun UNHP = UNIX HP PC = PC VMS = VMS	UNSU
Number of MCNP materials	integer	Number of materials from MCNP the user wants to have burned. This number must be <50.	3
MCNP material number	integer	The "m" number of the material(s) in the MCNP input file for which a burnup analysis is desired (all cells with this material(s) will be burned).	1 5 10
Material volume (cc)	real	Volume of cells in MCNP containing the aforementioned material number(s) (Note: if the user wants to use the volume calculated by MCNP, then 0.0 should be entered here).	0.0 0.0 0.0
Power (in MWt)	real	This is the total nominal power generated by the system represented in the MCNP input file.	1000.0
Recoverable energy per fission (in MeV)	real	If known, the recoverable energy per fission for the system (in MeV). (Note: if no value is known, then the value for ^{235}U preceded by a negative sign can be entered, and the Q-value will be determined using this number and the fraction of other actinides present).	-200.0
Total number of days burned	real	Indicates the length of time over which the entire irradiation will occur (Note: this value should be zero if a feed file is used and non-zero if one is not used).	0.0
Number of outer burn steps	integer	This value represents the number of times cross-section values for ORIGEN2 are updated by MCNP. When a feed file exists, it should be equal to the number of feed steps that exist in the feed input file.	7

TABLE 5 (cont)

		Additionally, each step may represent the addition or removal of more material, or it may just represent an additional timestep in irradiation periods. The number of outer burn steps must be <100.	
Number of internal burn steps	integer	This value gives the number of intervals into which the main irradiation period for each ORIGEN2 input file will be divided. The more internal burn steps, the more accurate the results from ORIGEN2. If continuous feed is being used, this value should be divisible by 10; otherwise, it should be divisible by 2.	40
Number of predictor steps	integer	Number of times MCNP and ORIGEN2 should be run halfway through each outer burn step (to correlate cross-section values with the composition of the system during burnup).	1
Step to restart after	integer	A value of 0 represents a new *monteburns* run. If it is greater than 0, then it indicates the number of a previously completed step after which new calculations will be performed. Note: Files containing information up to this outer burn step must already exist (in the user's working directory under the subdirectory tmpfile).	0
Number of ORIGEN2 library	10-char.	The two-digit identification number or name associated with the initial ORIGEN2 cross-section library.	60, Fftfc, or FFTFC
ORIGEN2 library location	72-char.	This is the path name of the ORIGEN2 libraries in the user's directory.	C:\origen 2\libs
Fractional importance limit	real	This value is the tolerance criteria used by *monteburns* to determine which isotopes from ORIGEN2 are "important" (see Section 3.4.6). "Important" isotopes are those for which the atom fraction, weight fraction, fraction of absorption, and/or fraction of fission in the overall material is greater than the limit listed	0.005

TABLE 5 (cont)

		here. If this value is less than zero, then those fission products that are not "automatically important" are lumped together as a general fission product in MCNP.	
Flag for intermediate k_{eff} calculations	integer	This value indicates whether or not intermediate MCNP run(s) are desired. If activated (=1) for discrete feed cases, MCNP will be run three times per burn step to get k_{eff} calculations before, after, and halfway through the step. If continuous or no feed exists, then MCNP is only run twice, once halfway through and once between burn steps. A value of 0 indicates only one MCNP run, which occurs halfway through each outer burn step.	0
Number of automatic tally isotopes and a list of those isotopes for each material	integer; for each isotope: first a five digit integer; then a period and a three digit identifier; 9-char. total	The number of isotopes for which the user specifies he/she wants to obtain tallies (no matter what the fractional importance the isotopes are). For each material, this number is then followed by a list of those isotopes according to their MCNP identifiers. Material 1 Material 5 Material 10	9 93237.55c 94238.50c 94239.55c 94240.50c 94241.50c 94242.50c 95241.50c 95242.50c 95243.50c 9 93237.55c 94238.50c 94239.55c 94240.50c 94241.50c 94242.50c 95241.50c 95242.50c 95243.50c 9 93237.55c 94238.50c 94239.55c 94240.50c 94241.50c 94242.50c 95241.50c 95242.50c 95243.50c

5.3.1. Basic Information

The following information about each outer burn must be included in the first block of data:

1. Step number
2. Irradiation time for each step
3. Fraction of total power at which the system will be operating during each burn step
4. Region in which each material will be located for the step
5. What feed group will be added to each material for the step (0 means no feed)
6., 7. Two feed rate columns
8. Number of the removal group number containing the elements that should be removed from ORIGEN2 output
9. What fraction of each element in this removal group should be removed

Items 5–7 will be discussed as part of the feed information and 8–9 as part of the removal information.

5.3.2. Feed Information

These variables comprise nine columns of data (see Table 5), which are read in free format. For burn steps where there is continuous feed, the first feed column (item 6) represents the feed rate (g / day) at the beginning of the step, and the second column (item 7) represents the feed rate at the end of the step. The exact rate of feed for each internal burn step is then obtained by interpolating between the beginning and ending feed rates. If a value of -1.0 is entered in the first feed rate column, then it is assumed that the beginning feed rate for that step is equal to the value of the ending feed rate of the previous step (thus, -1.0 cannot be entered as the beginning feed rate for the first step because it requires a previous step to obtain complete information). If the value entered in the first feed rate column is -2.0, then it indicates that discrete, not continuous, feed is added to the system at the beginning of the current outer burn step for this material. The amount of discrete feed added is equal to the value entered the second column (in grams / day) times the number of days in the irradiation. In either case, the user must enter the number of the feed material group he / she is adding for each outer burn step, or 0 if he / she is not adding any material.

5.3.3. Removal Information

Similarly, for the removal groups, the user must first enter the number of the removal group, followed by the fraction of each element in the removal group that should be removed (0.0 means that none of the element's inventory is removed, whereas 1.0 means the entire inventory of the designated elements is removed). If the removal group number is positive, then continuous removal occurs, whereas if it is negative, then discrete removal occurs. For discrete removal, *monteburns* edits the ORIGEN2 output file so that the desired fraction of the designated range(s) of elements is removed at the end of each outer burn step. For continuous feed, the fission products are removed by ORIGEN2 after the halfway predictor step as well as at the end of the burn step for each ORIGEN2 run. If the value of zero is entered for a feed or removal group, then no feed addition or removal occurs in that material during that outer burn step.

5.3.4. Feed Material Groups

The next block of information in the feed input file provides detailed data about the feed material groups. First, the user must list the number of feed material groups that he/she uses. Then, for each feed material group, he/she must list the number of isotopes in that feed group followed by identifiers for those isotopes and the mass fraction of feed each isotope contributes to the final feed material (these do not have to add up to one). The identifier includes the atomic number directly followed by the atomic mass number for each isotope (such as 92235 for ^{235}U).

5.3.5. Removal Groups

The final block of information describes the removal groups. Again, the user must first list the number of removal groups. Then, for each removal group, the user must list the number of ranges of consecutive elements that the removal group contains, followed by the atomic numbers of the first and last elements that comprise each range (all isotopes of the specified elements are in the removal group; i.e., individual isotopes may not be removed). For example, 28 to 68 would mean that all elements between nickel and erbium would be removed (which would represent the majority of fission products). The two ranges 28 to 42 and 44 to 68 would mean that all fission products in this same range, except technetium (Z=43), would be removed. The range 43 to 43 would indicate that the only element being removed would be technetium. For continuous removal (a removal group number >0), the appropriate elements would be removed both after the halfway predictor step and at the end of the burn (simulating continuous removal). For discrete removal (a removal group number <0), the elements are removed only at the end of the burn step (simulating discrete removal). In addition, ORIGEN2 has several different categories of isotopes: activation products, actinides, and fission products. The removal option in *monteburns* allows only isotopes generated as fission products to be removed, or it allows isotopes to be removed from all three categories. If the first integer in the range is listed as a positive number, isotopes of the element(s) listed in the removal group would be removed from all three categories. However, if this first integer is negative, then only isotopes of that

element(s) that has been produced as fission products would be removed (if a smeared region contains Zr clad, the user may wish to only process the Zr fission product from the waste while not removing the clad material).

5.3.6. Material Shuffling

Also in the feed input file, the user can specify if and/or how to shuffle materials between regions. *Monteburns* regions are defined according to the initial listing of MCNP materials to be burned in the *mbfile.inp* file. The volume (of the applicable MCNP cells) associated with the first MCNP material listed in the *mbfile.inp* file is designated as region 1, and so on. These region numbers remain unchanged throughout the entire calculation. The material contained in a *monteburns* region is given the same material number as the region number; for example, when the output refers to *monteburns* material 2, it refers to the material in region 2 for that burn step. Column 4 in the feed file input specifies which *monteburns* material is to be placed in each region prior to each burn step. In particular, the number in each region represents which region the current material was previously in. For example, if there are two regions to be burned, the first burn step would normally contain a "1" in column 4 for the first region and a "2" in column 4 for the second region; thus, the materials would remain as specified in the *mbfile.inp* file. If the user wants to exchange the materials between the two regions prior to the second burn-step, then he/she would enter a "2" in column 4 for the first region and a "1" in column 4 for the second region (again, regions are defined in the order in which volumes appear in the *mbfile.inp* file, and this same order must be followed in the feed input file).

5.3.7. Format of Files

Tables 6a and 6b display the format of two different feed input files. In the first example file (Table 6a), material is irradiated in region 1, moved from region 1 to region 2, and irradiated in region 2. Finally, the material is processed [all fission products except technetium (Tc) are removed and then transuranic actinides and Tc-99 are added] and reinserted into region 1. For all but the first step, feed material is added to the batch before entering region one (implied by a -2.0 in the first feed rate column), and in each step material is removed when the batch is pulled from region two (indicated by a negative removal group number). All fission products with an atomic number between 10 and 59 (with the exception of Tc) are removed and any isotope with an atomic number of 60 or 92 is removed (be it activation product, actinide, or fission product). The second example file (Table 6b) models continuous feed/removal of materials. In this case, plutonium is continuously added (at a decreasing rate) over the first five steps, whereas Tc is continuously removed. The feed is added continuously in ORIGEN2 over the burn period, and removal is performed by ORIGEN2 halfway through and at the end of each burn step (which in most *monteburns* cases will effectively simulate continuous removal). The -1.0 in the first feed rate column means that the beginning feed rate of the current step is the same as the ending feed rate of the previous step. If the feed rates at the beginning and end of the burn steps are different, then the feed rate used by ORIGEN2 is interpolated between these two values. The final two steps in Table 6b

are at zero power, which allows the material to decay with no irradiation involved. In addition to Tables 6a and 6b, another sample feed input file is included in Appendix E (which corresponds to the MCNP and *monteburns* input files in Appendices C and D, respectively).

5.3.8. Constant Burn Cases

If the user wants to perform a constant power burn with no material feed or removal, then he/she does not need to create a feed input file. Instead, a simple irradiation calculation would be performed in ORIGEN2 for the total length of irradiation (in days) listed in the *monteburns* input file (this value must be non-zero for such a case). The length of each outer burn step would then equal this value divided by the number of outer burn steps input.

5.4. Cross-section Map

The identifiers used to recognize isotopes in MCNP are different than those in ORIGEN2. Thus, *monteburns* is designed to determine which identifiers to use for each code. In ORIGEN2, the identifier is simply the atomic number followed by the atomic mass number and a "0" for stable isotopes and a "1" for metastable ones. MCNP not only requires the atomic number and atomic mass number but also a cross-section identifier. A file containing a list of default MCNP identifiers for all isotopes used or potentially created by decay or irradiation processes must be present in the directory in which the user is running so that *monteburns* knows what cross-sections to use. Note: cross-section libraries for many fission products may not exist and obviously cannot be listed here; they are subsequently ignored. This file is named *mbxs.inp* and can either be provided by the user or obtained with the source code and modified by the user as necessary. Each isotope must be listed on a separate line, and the values input here override those in the MCNP input file but do not override the ones listed in the *monteburns* input file.

For any isotopes deemed "important" by *monteburns* that do not have a cross-section identifier in this file, *monteburns* gives a warning that the cross-section is not found, continues to use the default ORIGEN2 cross-section, and does not transfer the material to MCNP. The identifiers in this file can either be cross-section libraries provided by MCNP, or they can be ones generated by the user with ENDF libraries, the code NJOY, and/or from other sources. In addition, *mbxs.inp* must include the general fission product identifiers 45117(.90c) and 46119(.90c) for MCNP if the lump sum of fission products option is used (as discussed in Section 4.2). A sample *mbxs.inp* file is displayed in Appendix F.

Versions of NJOY are available at the Radiation Safety Information Computational Center (RSICC) as codes PSR-171 and PSR-355.

TABLE 6a
DESCRIPTION/EXAMPLE 1 OF FEED INPUT FILE

Step #	Time step (days)	Fraction of Power	Material # in Each Region	Feed Group #	1st Feed Rate Column	2nd Feed Rate Column	Removal Group #	Removal Group Fraction
1	182.62	1.000	1 2	0 0	0.0 0.0	0.0 0.0	0 -1	1.000 1.000
2	365.25	1.000	2 1	1 0	-2.0 0.0	1250.0 0.0	0 -1	1.000 1.000
3	547.87	1.000	2 1	1 0	-2.0 0.0	1150.0 0.0	0 -1	1.000 1.000
4	730.50	1.000	2 1	1 0	-2.0 0.0	1070.0 0.0	0 -1	1.000 1.000
5	730.50	1.000	2 1	1 0	-2.0 0.0	1050.0 0.0	0 -1	1.000 1.000

Variable	Format	Example
Number of Feed Materials	i4	1
For Each Feed Material:		
Number of isotopes in feed	i4	12
Atomic Number / Atomic Mass Number of each isotope followed by weight fraction of that isotope in feed material (Note: this value does not have to add up to one. It can be fractionated however the user desires. For example, the numbers listed in the right-hand column add up to 1.31, but they are relative to each other and the total amount of grams / day of each isotope is equal to the value entered in the first block times this weight fraction regardless of whether it adds up to one or not.)	i5,f9.7	43099 0.310000 93237 0.044916 94238 0.014001 94239 0.514214 94240 0.237591 94241 0.078681 94242 0.048014 95241 0.051421 95242 0.000068 95243 0.009262 96243 0.000034 96244 0.001797
Number of Removal Groups	i4	1
For Each Removal Group:		
Number of Ranges for Group	i4	4
Range(s) of Atomic Numbers for Removal Group	i4,i4	-10 -42 -44 –59 60 60 92 92

TABLE 6b
EXAMPLE 2 OF FEED INPUT FILE

Step #	Time step (days)	Fraction of Power	Material # in Each Region	Feed Group #	1st Feed Rate Column	2nd Feed Rate Column	Removal Group #	Removal Group Fraction
1	182.62	1.000	1	1	1400.0	1300.0	1	1.000
2	365.25	1.000	1	1	-1.0	1250.0	1	1.000
3	547.87	1.000	1	1	-1.0	1150.0	1	1.000
4	730.50	1.000	1	1	-1.0	1070.0	1	1.000
5	730.50	1.000	1	1	-1.0	1050.0	1	1.000
6	365.25	0.000	1	1	0.0	0.0	0	0.000
7	365.25	0.000	1	1	0.0	0.0	0	0.000

Variable	Format	Example
Number of Feed Materials	i4	1
For Each Feed Material:		
Number of isotopes in feed	i4	2
Identifier / Weight Fraction	i5,f9.7	94239 0.94 94240 0.06
Number of Removal Groups	i4	1
For Each Removal Group:		
Number of Ranges	i4	1
Range	i4,i4	43 43

6.0. ERROR MESSAGES

There are a number of problems that can occur in *monteburns*, some of which may be caused by errors in the user's input files. Many such errors are accompanied by warning or error messages that appear on the screen (with the exception of one, which appears in the file T9err_#) to notify the user of the potential problem(s). These messages are listed and described in Table 7.

TABLE 7
ERROR MESSAGES

Error Message	Cause
***** MB ERROR: You must uncomment certain lines at the top of the source code for this operating system	Different operating systems have different system-dependent calls for obtaining arguments on the command line. This error occurs when the operating system specified in input is not consistent with the FORTRAN executable (a compilation error should also occur in this case).
***** MB ERROR: Problem with *monteburns* input file	The *monteburns* input file was not read in correctly. Please check your file for formatting and try again.
***** MB ERROR: No tally volume	If the user inputs a material volume of 0.0 in the ***.inp file, then the volume of the MCNP material must be obtained by adding up the volume of each cell containing that material in the MCNP output file. If MCNP contains no value for any cells containing that material, then this error message will appear. Because this volume is used in energy spectrum and cross-section tally calculations, *monteburns* will terminate after displaying this error message if the volume is zero.
***** MB WARNING: Natural iso xs not found #####	The MCNP cross-section libraries used in this program only have a limited number of values for natural elements. If the natural element entered by the user is not found in the cross-section library used in this program, then this error message appears and the element will not be included in the MCNP input files. The cause of this error could either be that the user forgot to put the natural element cross-section in *mbxs.inp* or that it does not exist in MCNP (in which case the MCNP input file would not work anyway).
***** MB WARNING: Iso xs not found #####	This warning message appears when the cross-section for one of the isotopes originally found in the MCNP input file cannot be found in the file *mbxs.inp* (the user should add it to this file).
***** MB ERROR: Initial ORIGEN2 library was not found	The ORIGEN2 library specified by the user (for initial cross-sections) was not found on the system (see Section 4.2.2).
***** MB ERROR: Invalid removal group entered for outer step number #	In the feed input file, the user must enter the number of the removal group associated with each outer burn step. Additionally, he/she must also enter the number of removal groups in the final block along with the atomic number of element ranges in the removal groups. If the user enters a removal group number greater than the value of the number of removal groups, then this error message

TABLE 7 (cont)
ERROR MESSAGES

Error Message	Cause
	appears on the screen and *monteburns* stops running (# stands for the outer burn step number).
***** MB ERROR: Problem with feed input file	The feed input file was not read in correctly. Please check your file for formatting and try again.
***** MB ERROR: Not all user-specified MCNP materials were found in MCNP output file	In the *monteburns* input file (***.inp), the user must specify which material(s) from MCNP he/she wishes to have burned (i.e., transferred between ORIGEN2 and MCNP). If one or more of these materials are not found in the MCNP output file, then this error message will appear on the screen and *monteburns* will terminate
***** MB ERROR: Tally read error	This means that the flux tally value from an MCNP output file was read as zero. A flux value of zero is then transferred to an ORIGEN2 input file, which means that no burnup will occur. Nonetheless, *monteburns* does not stop running.
***** MB ERROR: Cross-section Tallies Not Correct	If there are not enough tally output results in the MCNP output file for the number of tallies needed, then this error message will occur. It typically indicates a problem with the MCNP run. This error could be caused by tallies that existed in the initial MCNP deck (if they were numbered >100), or if the user exceeds the maximum allowable material limits.
***** MB WARNING: Isotope ##### not found in TAPE9.INP	There are some fission and activation products produced during the irradiation of a material that do not have cross-section values in the working ORIGEN2 cross-section file. Thus, their fraction importance in the areas of absorption and fission contribution cannot be calculated (although atom and weight fraction are). These fission and activation products are listed with this warning message in the file "tmpfile/T9err_$" ($ is the *monteburns* material number). Although not necessarily a concern, these should be noted.
***** MB WARNING: mcnp xs not found #####	The MCNP cross-section libraries used in this program have a limited number of isotopes for which cross-section values exist. If an isotope is determined by *monteburns* to be "important," but its cross-section identifier for MCNP does not exist in the file *mbxs.inp*, then this warning message appears and the isotope is not transferred back to MCNP. This message may also appear if an isotope from a natural element in the initial MCNP input is found to be

TABLE 7 (cont)
ERROR MESSAGES

Error Message	Cause
	"important" but does not have a cross-section because it is a natural element. It is then typically included in the MCNP input file as part of the natural element.
***** MB WARNING: No Uranium (or Plutonium) Fission Product library was provided in mbxs.inp	If the fractional importance value is negative, then fission products resulting from ORIGEN2 irradiation calculations (except those deemed "important") are summed together and given two general MCNP cross-sections for fission products (the total sum is divided according to the percent of fissions caused by ^{235}Uand ^{239}Pu and given the appropriate cross-section for each). If either of these two fission product cross-section libraries are not included in *mbxs.inp*, then this message appears and they are neglected.

7.0. OUTPUT FILES

Two large, primary output files are produced by *monteburns*. These output files consist of the name of the MCNP input file created by the user followed either by the extension *".out"* or *".chk."* For each of the output groups listed below (except the first two, which contain system, not material dependent parameters), results appear for each *monteburns* material/region being analyzed. Note: this is not necessarily the same as the initial MCNP material number assigned to each region because of shuffling between regions. The user must keep track of each MCNP material individually through the various regions when shuffling occurs. A sample *.out* file is included as Appendix G.

The first output file, *mbfile.out*, contains the results displayed below for each outer burn step.

- ***Monteburns* MCNP k_{eff} Vs Time**—a list of the cumulative time (in days) over which irradiation has occurred as well as the effective multiplication factor (k_{eff}), associated relative error, υ [Eqs. (8) or (9)], average recoverable energy per fission calculated by *monteburns* [Eqs. (1–4)], and η for the system (Eq. 10).

- ***Monteburns* MCNP k_{eff} at Beginning of Step**—a list of the cumulative time of irradiation (in days) that has occurred before each step begins as well as the effective multiplication factor, relative error, and υ at the beginning of each outer burn step (after discrete feed occurs). These data

are only included in the output if discrete feed is used and intermediate k_{eff} calculations are requested.

For each material and outer burn step, the following parameters are output.

- ***Monteburns* Transport History**—the recoverable energy per fission (Eq. 1), neutron flux (Eq. 5), macroscopic fission cross-section (Σ_f), power generation, burnup [in gigawatt-days per metric ton heavy metal (i.e., actinides) (GWd/MTHM)], capture - (n,γ), fission - (n,f), and (n,2n) cross-sections, fission-to-capture ratio, and η (Eq. 10) for both the material as a whole and the actinides only.

- ***Monteburns* Flux Spectrum**—the percent of neutrons with energies in each of the following ranges: 0 to 0.1 eV, 0.1 to 1 eV, 1 to 100 eV, 100 eV to 100 keV, 100 keV to 1 MeV, and 1 MeV to 20 MeV. To obtain a more detailed spectrum, the user must enter his/her own tallies into the MCNP input file or modify *monteburns* to provide the values desired.

The following results are provided for each "automatic" isotope in each material for each outer burn step

- ***Monteburns* One-Group (n,γ) Cross-sections**—the value of the microscopic (n,γ) capture cross-section (σ_c). Other reactions, (n,2n), (n,3n), (n,α), and (n,p) are also calculated by *monteburns* for certain isotopes, but they are not listed in the output. If desired, these cross-sections can be found in the modified TAPE9.INP ORIGEN2 libraries.

- ***Monteburns* One-Group Fission Cross-sections**—the value of the microscopic fission cross-section (σ_f).

- ***Monteburns* Fission-to-Capture Ratio**—the ratio of the microscopic fission cross-section to the microscopic capture (n,γ) cross-section (σ_f / σ_γ) [does not include (n,α), (n,p), etc].

- ***Monteburns* Grams of Material at Beginning of Steps**—this represents the amount of material (in grams) that exists in the system at the beginning of each step.

- ***Monteburns* Grams of Material at End of Steps**—the amount of material (in grams) at the end of each step.

- ***Monteburns* Grams of Feed**—the amount of material (in grams) added to the system.

- ***Monteburns* Grams Produced (or Destroyed)**—the amount of material (in grams) produced (or destroyed if the output is negative) during irradiation. The interpretation of this data may depend on feed, removal, and/or material shuffling.

- **Summary of Inventory/Feed/Production**—the total amount of material in the system at the beginning and end of *monteburns* (not of each step), the amount added through feed, and the net change. The interpretation of these data may also depend on feed, removal, and/or material shuffling.

- **Feed Rate**—the average continuous feed rate (in grams per day).

- **Production/Destruction Rate**—the rate of change (in grams per day) of material produced to that destroyed during irradiation. The interpretation of these data may depend on feed, removal, or material shuffling.

- ***Monteburns* Activity of Material at End of Steps**—the activity (in Curies) of each isotope [Eq. (18)].

- ***Monteburns* Heatload of Material at End of Steps**—the decay power (heatload in W) of each isotope (Eq. 20).

- ***Monteburns* Inhalation Toxicity at End of Steps**—the inhalation toxicity of a nuclide in the air (m^3 air) as shown in Eq. (21). This represents the biological hazard the material presents to a human who is near enough to inhale it (i.e., sensitivity of the human to that material).

- ***Monteburns* Ingestion Toxicity at End of Steps**—the ingestion toxicity of a nuclide in water (m^3 water) as shown in Eq. (22). Again, this represents the biological hazard the material presents to a human who is near enough to ingest it (i.e., sensitivity of the human to that material).

- **Feed Input File**—if it exists, this file is included at the end of this output file so that the user can determine what feed parameters he/she used to produce the results presented in this output file.

In the second output file, *mbfile. chk*, many intermediate results from the execution of *monteburns* are listed. In this output file, the following results are reported for each *monteburns* material analyzed for each predictor step.

- ***Monteburns* Spectrum for Each Predictor**—the percent of neutrons with energies in each of the following ranges: 0 to 0.1 eV, 0.1 to 1 eV, 1 to 100 eV, 100 eV to 100 keV, 100 keV to 1 MeV, and 1 to 20 MeV. This can be

used to determine if smaller time intervals or more predictor steps need to be run.

- ***Monteburns* Grams at Midpoint**—the amount of each isotope (in grams) present halfway through the irradiation for both the predictor and the actual steps. The grams of each automatic "important" isotope present halfway through each predictor step are listed first for each outer burn step followed by the composition of these isotopes halfway through the actual step. This way the user can determine if the predictor step(s) provided enough accuracy or if more predictor steps (or smaller time intervals) are needed. If the two values for any isotope are significantly different, then *monteburns* should be rerun using more predictor steps or outer burn steps to obtain more representative cross-sections.

- **Importance Fraction of Isotopes Sent from ORIGEN2 to MCNP**—the isotopes deemed "important," both automatically and through the importance fraction. This list contains the total mass of the isotope in the specified region and the contribution of each isotope in the following four categories: absorption, fission, mass fraction, and atom fraction. For example, if the fission column for an isotope reads 0.1, then 10% of the overall fissions in the material resulted from this isotope. This file also includes a warning message if an isotope deemed "important" by *monteburns* or "automatic" by the user is not found in the MCNP cross-section library used by *monteburns*.

8.0. LIMITATIONS OF AND FUTURE WORK FOR *MONTEBURNS*

Monteburns is only as good as the MCNP cross-sections that are available to the user. If cross-section libraries do not exist for several fission products or actinides, or cross-sections at the appropriate temperatures are not available, then *monteburns* results should be closely scrutinized. *Monteburns* is also limited by the accuracy of the ORIGEN2 fission product yields.

Monteburns output only contains data relating to material isotopics and a few reactor physics parameters (k_{eff}, η, υ, etc.). It can be modified in the future, however, to extract more values, depending on what uses the program might eventually have.

Monteburns currently uses the most simple form of the predictor-corrector method. In the future a more sophisticated numerical technique could be applied, although the simple method has proven adequate for problems studied thus far.

Monteburns currently uses ORIGEN2.1. There may be some advantages to using ORIGEN-S or CINDER[5] in the future because of increased output options, improved default cross-section sets and fission product yields, and possibly wider availability.

Monteburns cannot currently handle any neutron reaction other than (n,γ), (n,f), (n,2n), (n,3n), (n,α), and (n,p). Any application that relies significantly on any other reaction [for example, (n,t) in Li^6] will not work correctly.

Monteburns does not currently work with the Lahet Code System (LCS) or MCNPX. For now, accelerator-driven systems need to be evaluated with a MCNP "sdef" source definition. Test problems have shown that an evaporation source with a proper geometric distribution produces results similar to a full-blown, high-energy neutron solution (for systems with reasonably high neutron multiplication). Because of the lack of high-energy capability, *monteburns* does not handle spallation products.

As mentioned in Section 3.4.1, *monteburns* could do a better job of calculating changes in Q_{fis} as the system burns. Future modifications may look at adding the necessary tallies to better estimate Q_{fis} (to include the energy deposition from fission gammas, capture gammas, and neutron kinetic energy).

More detailed benchmarking efforts also need to be performed. Although two-dimensional reactor systems have been benchmarked to SCALE runs,[9,3] three-dimensional systems need to be studied in more detail.

In addition to the possible modifications above, work is ongoing to make the input/output of *monteburns* more user-friendly. Also, work is continuing in the benchmarking of *monteburns* to experimental and analytical burnup results, as well as for a wide range of inputs.

Any problems not already addressed should be reported to the contacts in Section 1.1 so that they can be corrected.

9.0. IMPLEMENTATION OF *MONTEBURNS*

The *monteburns.pl* executable can be run on almost any platform as long as the following files are present in the working directory and the directory has access to Perl, MCNP, and ORIGEN2 (including the libraries). The symbol '*mbfile*' represents the name the user assigns to the input files (Note: all three input files must have the same name with different extensions).

- *Mbfile*—MCNP input file
- *mbfile.inp*—user's input file
- *mbfile.feed* (optional)—feed input file
- *mbxs.inp*—MCNP cross-section file
- *monteb* or *monteb.exe* (FORTRAN77 executable) and/or *monteb.f* (FORTRAN77 program)
- *monteburns .pl*—Perl script file

9.1. UNIX

To run *monteburns.pl* on a UNIX system, the user must have a copy of *monteburns.pl* and either the executable FORTRAN77 program *monteb* that is operable on his/her system or compile the executable from the FORTRAN77 program *monteb.f*. The FORTRAN77 program can be compiled using the following command.

```
% f77 -o monteb monteb.f
```

Note: when using an HP system, there are several lines at the beginning of the monteb.f file that must be commented out (these are clearly marked within the first 25 lines of *monteb.f*), and some that must be uncommented before it will compile.

Alternatively, an executable for both UNIX systems (Sun and HP) is available with the source code as *monteb* and *monteb.hp* respectively.

Monteburns can then be run by typing the following command at the UNIX prompt.

```
% monteburns.pl
```

If the user obtains a "permission denied" message, then make the file an executable with the following command.

```
% chmod +x monteburns.pl
```

Once it is running, the basename of the input files will be requested with the following line: "Enter base name of input files."

After entering this information (i.e., the name *mbfile*), *monteburns* should be running with messages printed to the screen telling the user at which step in execution he/she is. A log file of detailed information, *log.txt*, will also be produced, which is helpful in determining what went wrong in a "bad" run.

9.2. PC

Running *monteburns* on the PC is almost identical to UNIX except that the executable is called *monteb.exe*. If the user wishes to compile on the PC, then he/she must use a compiler that handles the "getarg" function (i.e., Digitial Developer Studio 5.0 or 6.0 or others, not Lahey). To run in a windows environment, the user can simply click on the executable *monteburns.pl*. In a DOS environment, the program can again be run by typing "monteburns.pl." *Monteburns* has been tested on a Windows NT platform and should work on other Windows systems, but this cannot be guaranteed.

9.3. VMS

Running *monteburns* on a VMS system is similar to UNIX except that again, there are several lines at the beginning of the *monteb.f* file that must be commented out and some that must be added (what is there for VMS may or may not work correctly). The details necessary for this system were not yet identified when this manual was published, so any user that wants to use this system may have to do a little manipulation. Please contact the authors during or after this process so the capability may become available to others (or check with RSICC to see whether or not it was done yet).

10.0. REFERENCES

1. Judith F. Briesmeister, Ed., "MCNP™—A General Monte Carlo N-Particle Transport Code, Version 4B," Los Alamos National Laboratory document LA-12625-M (March 1997).

2. RSICC Computer Code Collection, "ORIGEN2.1; Isotope Generation and Depletion Code, Matrix Exponential Method," Oak Ridge National Laboratory document CCC-371 (December 1991).

3. RSICC Computer Code Collection, "SCALE4.3: Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation for Workstations and Personal Computers, Volume 2, Part 1," Oak Ridge National Laboratory document CCC-545 (December 1991) p. F7.2.1-3.

4. John R. LaMarsh, *Introduction to Nuclear Engineering*, 2nd ed. (Addison-Wesley Publishing Company, Reading, Massachusetts, 1983) pp. 77, 104.

5. W. B. Wilson et al., "Accelerator Transmutation Studies at Los Alamos with LAHET, MCNP, and CINDER'9*0*," Proceedings of the Workshop on Simulation of Accelerator Radiation Environments, January 11–15, 1993, Santa Fe, New Mexico. Los Alamos National Laboratory document LA-12835-C (October 1994) pp.115–133.

6. M. Benedict, T. H. Pigford, and H. W. Levi, *Nuclear Chemical Engineering* (Mc-Graw Hill Book Company, New York, 1981) pp. 363–364, 979–981.

7. J. E. Turner, *Atoms, Radiation, and Radiation Protection* (McGraw-Hill, Inc., New York, 1992) p. 64.

8. A. G. Croff, "A User's Manual for ORIGEN2 Computer Code," Oak Ridge National Laboratory document ORNL/TM-7175 (July 1980).

9. H. R. Trellue, "Development of Monteburns: a Code that Links MCNP and ORIGEN2 in an Automated Fashion for Burnup Calculations," Los Alamos National Laboratory document LA-13514-T (December 1998).

11.0. APPENDICES

See the enclosed appendices.

APPENDIX A - MCNP Input File – test1

```
Heatpipe power system - Nb1Zr clad UN, flat/flat=20.1cm. length=31cm
c   Passively safe: radref on, drums in, flooded, wet sand surround
c   Passively safe: radref off, flooded, wet sand surround
c   Passively safe: radref off, flooded, water surround
c
101 0           -401  402 -403  404 -405  406  $ Core (fill=1)
                 203 -206  fill=1  imp:n=1
102  8  -8.64   -411  412 -413  414 -415  416  $ Hex
                (401:-402:403:-404:405:-406)
                 203 -206  imp:n=1
103  0          -441  442 -443  444 -445  446  $ Gap
                (411:-412:413:-414:415:-416)
                 203 -206  imp:n=1
110  8  -8.64   -411  412 -413  414 -415  416  206 -207  imp:n=1 $ Nb Plate
112  8  -8.64   -411  412 -413  414 -415  416  202 -203  imp:n=1 $ Nb plate
113  0          -411  412 -413  414 -415  416  222 -202  imp:n=1 $ Void
114  8  -8.64   -411  412 -413  414 -415  416  201 -222  imp:n=1 $ Gamma Core
115  8  -8.64   -250  200 -201                           imp:n=1 $ Gamma ref
c
c      Shield
120 12 -7.9     -250 -260  199 -200  imp:n=1 $ imp:p=4 $ SS Clad
121 20 -1.093   -250 -260  198 -199  imp:n=1 $ imp:p=4 $ LiH
122 20 -1.093   -250 -260  197 -198  imp:n=1 $ imp:p=8 $ LiH
123 20 -1.093   -250 -260  196 -197  imp:n=1 $ imp:p=8 $ LiH
c
c     124 5 -10.1     -250 -260  195 -196  imp:n=1  $  imp:p=16 $ W
c
124 20 -1.093   -250  195 -196      imp:n=1  $ imp:p=16 $ LiH
125 20 -1.093   -250 -260  194 -195  imp:n=1 $ imp:p=16 $ LiH
126 20 -1.093   -250 -260  193 -194  imp:n=1 $ imp:p=32 $ LiH
127 20 -1.093   -250 -260  192 -193  imp:n=1 $ imp:p=32 $ LiH
128 12 -7.9     -250 -260  191 -192  imp:n=1 $ imp:p=32 $ SS
131 0           -250 -260  190 -191  imp:n=1 $ imp:p=32 $ DummyVoidPastShield
132 0           -250  260 -200  190  imp:n=1 $ imp:p=32 $ Void outside taper
133 0                -190  189 -104  imp:n=1 $ imp:p=32 $ Void to dose plane
134 0                -189  188 -104  imp:n=1 $ imp:p=32 $ Void past dose plan
c
c      Flood Zones
141  0          (441:-442:443:-444:445:-446)   $ Void below RR
                -102  203 -213   imp:n=1
142  0          (441:-442:443:-444:445:-446)   $ Void above RR
                -102 -250  216 -206   imp:n=1
143  0          -102 -250  207 -208   imp:n=1  $ Bot Flood
144  0          (102:250) -103  201 -208       $ Radial Flood
                 #831 #832 #833 #834 #835 #836 imp:n=1
145  0          (411:-412:413:-414:415:-416)   $ Rad Plate Flood
                  -102 -250  201 -203   imp:n=1
146  0          (411:-412:413:-414:415:-416)   $ Rad Plate Flood
                  -102 -250  206 -207   imp:n=1
c
c      Kill Zones
151 0            250 -103  190 -201   imp:n=0     $ Void outside shield cone
152 0            103 -104  190 -208   imp:n=0     $ Void oustide flood zone
153 0            104:-188:208         imp:n=0
c
c     Rad Ref and Control
```

```
801  8  -8.64   -451  452 -453  454 -455  456  $ Nb1Zr RR Inner Liner
               (441:-442:443:-444:445:-446)
                213 -216  imp:n=1
802  8  -8.64   (248:101) -102  213 -216 -250  $ Nb1Zr RR Outer Liner
                #831 #832 #833 #834 #835 #836 imp:n=1
811  3  -2.86   -101 -248  213 -216  702 -703 #831  $ Rad Ref 1
               (451:-452:453:-454:455:-456)  imp:n=1
812  3  -2.86   -101 -248  213 -216  704  705 #832 $ Rad Ref 2
               (451:-452:453:-454:455:-456)  imp:n=1
813  3  -2.86   -101 -248  213 -216  702 -706 #833 $ Rad Ref 3
               (451:-452:453:-454:455:-456)  imp:n=1
814  3  -2.86   -101 -248  213 -216 -701  704 #834 $ Rad Ref 4
               (451:-452:453:-454:455:-456)  imp:n=1
815  3  -2.86   -101 -248  213 -216 -706 -703 #835 $ Rad Ref 5
               (451:-452:453:-454:455:-456)  imp:n=1
816  3  -2.86   -101 -248  213 -216  705 -701 #836 $ Rad Ref 6
               (451:-452:453:-454:455:-456)  imp:n=1
821  8  -8.64   -101 -248  701 -702  213 -216  $ Rad Ref Clad
               (451:-452:453:-454:455:-456)  imp:n=1
822  8  -8.64   -101 -248  703 -704  213 -216  $ Rad Ref Clad
               (451:-452:453:-454:455:-456)  imp:n=1
823  8  -8.64   -101 -248  705 -706  213 -216  $ Rad Ref Clad
               (451:-452:453:-454:455:-456)  imp:n=1
824  8  -8.64   -101 -248 -701  702  213 -216  $ Rad Ref Clad
               (451:-452:453:-454:455:-456)  imp:n=1
825  8  -8.64   -101 -248 -703  704  213 -216  $ Rad Ref Clad
               (451:-452:453:-454:455:-456)  imp:n=1
826  8  -8.64   -101 -248 -705  706  213 -216  $ Rad Ref Clad
               (451:-452:453:-454:455:-456)  imp:n=1
832  0          -154  213 -214 fill=8 imp:n=1     $ Ctr Dm 1
833  like 832 but *trcl=(0 0 0  60  30 90  150  60 90)
834  like 832 but *trcl=(0 0 0 120  30 90  150 120 90)
835  like 832 but *trcl=(0 0 0 180  90 90   90 180 90)
836  like 832 but *trcl=(0 0 0 120 150 90   30 120 90)
831  like 832 but *trcl=(0 0 0  60 150 90   30  60 90)
c
851  15 -2.30   150 -151  155  156    u=8 imp:n=1 $ B4C  Ring
852  66 -12.65  151 -152  155  156    u=8 imp:n=1 $ Mo/Re Ring
853  15 -2.30   152 -153  155  156    u=8 imp:n=1 $ B4C  Ring
854  3  -2.86   -153 #851 #852 #853   u=8 imp:n=1 $ Inner CD
855  0           153                  u=8 imp:n=1 $ Gap
c
c     Hex and Pins (or empty hexes)
201 0            -301  302 -303  304 -305  306
                  lat=2  u=1  imp:n=1
                   fill=-5:5 -5:5 0:0
              9 9 9 9 9 9 9 9 9 9 9
              9 9 9 9 9 4 2 4 4 4 9
              9 9 9 9 4 4 4 4 2 4 9
              9 9 9 4 2 4 2 4 4 4 9
              9 9 4 4 4 4 4 4 2 4 9
              9 4 2 4 4 7 4 4 4 4 9
              9 4 4 2 4 4 2 4 2 9 9
              9 4 4 4 4 4 4 4 9 9 9
              9 2 4 2 4 2 4 9 9 9 9
              9 4 4 4 4 4 9 9 9 9 9
              9 9 9 9 9 9 9 9 9 9 9
c
```

```
c     UN Region HP
160  0           -511            u=2 imp:n=1   $ HP Void
161  8  -8.64     511 -503        u=2 imp:n=1   $ Nb HP
168  17 -3.59     503             u=2 imp:n=1   $ Interstitial
c     UN Pin
180  1 -13.56    -501  204 -205  u=4 imp:n=1   $ Fuel Pellet
181  3  -2.86    -501 -204       u=4 imp:n=1   $ Ax Ref Pellet
182  3  -2.86    -501  205       u=4 imp:n=1   $ Ax Ref Pellet
183  0           501 -502        u=4 imp:n=1   $ Gap
184  7  -20.     502 -504       u=4 imp:n=1   $ Re Liner
185  8  -8.64     504 -503        u=4 imp:n=1   $ Nb Clad
192  17 -3.59     503             u=4 imp:n=1   $ Interstitial
c     Flux Trap
401  0           -512            u=7 imp:n=1   $ Inner Void
402  15 -2.3      512 -511        u=7 imp:n=1   $ B4C
403  6  -10.20    511 -503        u=7 imp:n=1   $ Mo/Re Pipe
404  17 -3.59     503             u=7 imp:n=1   $ Interstitial
c     BeO Pin
510  3  -2.86    -501            u=3 imp:n=1   $ BeO Pellet
511  0           501 -502        u=3 imp:n=1   $ Gap
512  8  -8.64     502 -503        u=3 imp:n=1   $ Nb Clad
517  17 -3.59     503             u=3 imp:n=1   $ Interstitial
c     Void, No Tube
601  8  -8.64    -599            u=9 imp:n=1   $ Nb Slats
c

c
c     Surface Cards
101  cz  19.97     $ Rad Ref
102  cz  20.07     $ Nb-1Zr Liner
103  cz  40.55     $ Flood Plane
104  cz  185.00      $ Dose circle
c
188  pz -1200.1      $ Just past dose plane
189  pz -1200.0      $ Dose plane
190  pz -72.40      $ Dummy void to allow tally
191  pz -71.40      $ SS Clad
192  pz -71.20      $ LiH
193  pz -65.20      $ LiH
194  pz -59.20      $ LiH
195  pz -53.20      $ LiH
196  pz -47.20      $ LiH
197  pz -41.20      $ LiH
198  pz -35.20      $ LiH
199  pz -30.20      $ SS Clad
200  pz -30.00      $ Thin gamma ref plate
201  pz -29.50      $ Thick gamma core
222  pz -27.50      $ Void
202  pz -21.50      $ Nb Plate
203  pz -21.00      $ Ax Ref
204  pz -16.00      $ Shield end of core
205  pz  16.00      $ Nozzle end of core
206  pz  21.00      $ Ax Ref
207  pz  21.50      $ Nb Plate
208  pz  34.00      $ Flood
213  pz -18.00      $ Bot Rad Ref
214  pz  16.00      $ Top of CD
216  pz  18.00      $ Top Rad Ref
```

```
248  kz  327.0 .0042  $ RR BeO Cone
250  kz  330.0 .0042  $ Dose Cone
260  kz  -89.00  1.0   $ HP Cone
c
c    Control Drum (120deg)
150  c/z  0   15.72 2.75
151  c/z  0   15.72 3.65
152  c/z  0   15.72 3.85
153  c/z  0   15.72 4.75
154  c/z  0   15.72 4.80
155  p  -0.57735  1  0    15.72
156  p   0.57735  1  0    15.72
c
c     Fuel pin hex
301  px  1.27                   $ Flat to center
302  px -1.27
303  p   .57735  1  0   1.46647
304  p   .57735  1  0  -1.46647
305  p  -.57735  1  0   1.46647
306  p  -.57735  1  0  -1.46647
c
c     Baffle inner planes
401  py  10.0688
402  py -10.0688
403  p  1.73205  1  0   20.1376
404  p  1.73205  1  0  -20.1376
405  p -1.73205  1  0   20.1376
406  p -1.73205  1  0  -20.1376
c     2mm baffle planes
411  py  10.2688
412  py -10.2688
413  p  1.73205  1  0   20.5376
414  p  1.73205  1  0  -20.5376
415  p -1.73205  1  0   20.5376
416  p -1.73205  1  0  -20.5376
c     RadRef Nb1Zr (1mm gap)
441  py  10.3688
442  py -10.3688
443  p  1.73205  1  0   20.7376
444  p  1.73205  1  0  -20.7376
445  p -1.73205  1  0   20.7376
446  p -1.73205  1  0  -20.7376
c    Rad Ref
451  py  10.4688
452  py -10.4688
453  p  1.73205  1  0   20.9376
454  p  1.73205  1  0  -20.9376
455  p -1.73205  1  0   20.9376
456  p -1.73205  1  0  -20.9376
c
c     Fuel pin dimensions
501  cz  1.1350     $ Pellet
502  cz  1.1500     $ Gap
503  cz  1.2699     $ Clad
504  cz  1.2100     $ Re Liner
511  cz  1.1501     $ Inner HP wall
512  cz  1.1100     $ B4C Flux Trap Liner
599  cz  1.9999     $ Empty Hex Shell
```

```
c
c      Rays Defining Radref sections
701  py -.1
702  py  .1
703  p  -1.73205  1  0  -.2
704  p  -1.73205  1  0   .2
705  p   1.73205  1  0   .2
706  p   1.73205  1  0  -.2

c
c     UN TD=14.123 / 96%=13.56 (97.6 enr)
m1    92235.50c 0.488  92238.50c 0.012 7014.50c 0.5  $UN
c
c     BeO TD=3.01 / 95%=2.86
m3   4009.50c 0.5  8016.50c 0.5                      $BeO
mt3  beo.06t
c
c     Mo-Re TD=10.20
m6   42000.50c  1.000                                 $Mo
c     75185.50c  .120  75187.50c  .180
c
c     Mo-25Re TD=12.65
m66   42000.50c  .750                                 $Mo25Re
      75185.50c  .100  75187.50c  .150
c
c     Re  TD=20
m7   75185.50c  .4      75187.50c  .6               $Re
c
c     Nb1Zr  TD=8.64
m8   41093.50c  .99     40000.56c  .01              $Nb1Zr
c
c     H2O
c  m10   1001.50c  2        8016.50c  1               $ H2O
c  mt10  lwtr.01
c
c     Wet Sand  TD=2.05 (63.636%quartz)
c  m11   1001.50c  0.72727                           $ Wet sand
c        8016.50c  1.63636
c       14000.50c  0.63636
c  mt11  lwtr.01
c
m12  42000.50c -0.02               $ 316L Stainless
     24000.50c -0.16               $  (7.9g/cc)
     26000.55c -0.72
     28000.50c -0.10
c
c     B4C  TD=2.3 (90%enr)
m15   5010.50c  .720                              $B4C
      5011.50c  .080
      6000.50c  .200
c
c     Ints Mat 3%B4C TD=7.98g/cc, 45%=3.59g/cc
m17   41093.50c  -.97  5010.50c -.0231  6000.50c -.0069
c
c      Natural LiH with about 5 Vol% SS
m20   42000.50c  8.4e-5              $
      24000.50c  6.7e-4
      26000.55c  3.02e-3
```

```
      28000.50c  4.2e-4
      1001.50c   .05326
      3006.50c   3.994e-3
      3007.50c   0.04926
c
c     Flooded Ints Mat 3%B4C 45%Nb+55%H20=4.14g/cc
c  m97   41093.50c -.8410  5010.50c -.0200  6000.50c -.0060
c         1001.50c -.015   8016.50c -.118
c  mt97   lwtr.01
c
print
prdmp 100 5 0 1
mode n
kcode 1000 1.0 5 55
ksrc  6 0 9  6 0 -9  -6 0 9  -6 0 -9
```

End of Appendix A

APPENDIX B - Monteburns Input File With No Feed– test1.inp

```
Heatpipe Power System (HPS) 12 module core, 10 yr burn @ 750 kW
UNSU       ! Type of Operating System
1          ! Number of MCNP materials to burn
1          ! MCNP material number #1 (will burn all cells with this mat)
6022.      ! Material #1 volume (cc), input 0 to use mcnp value (if exists)
0.80       ! Power in MWt (for the entire system modeled in mcnp deck)
-200.      ! Recov. energy/fis (MeV); if negative use for U235, ratio other isos
3652.0     ! Total number of days burned (used if no feed)
4          ! Number of outer burn steps
40         ! Number of internal burn steps (multiple of 10)
1          ! Number of predictor steps (+1 on first step), 1 usually sufficient
0          ! Step number to restart after (0=beginning)
60         ! number of default origen2 lib - next line is origen2 lib location
/export/gus2/origen/libraries
.001       ! fractional importance (track isos with abs,fis,atom,mass fraction)
0          ! Intermediate keff calc. 0) No 1) Yes
6          ! Number of automatic tally isotopes, followed by list.
92235.50c
92238.50c
94239.55c
94240.50c
94241.50c
94242.50c
```

End of Appendix B

APPENDIX C - MCNP Input File – test5

(Note: this is the same as the "test3" file included with the source code but has better statistics (i.e., processes more particles), so results will vary somewhat)

```
adv1c  Advanced ATW, 2mDiamx2mHigh, 2 GW, 0.5mTarg, Equil,
c      Fuel - PWR mix
c
100     2 -10.242  100 -120 -204        imp:n=1         $ Lead
120     2 -10.242  120 -130 -200        imp:n=1         $ Lead Below Target
140     2 -10.242  130 -131 421 -200    imp:n=1         $ Lead Target
141     2 -10.242  130 -131 -421        imp:n=1         $ B4C Insert
150    20 -7.9     131 -132 -200        imp:n=1         $ Target Window
260     0          132 -160  421 -200   imp:n=1         $ Void Above Lead
Target
261     0          132 -160 -421        imp:n=1         $ B4C Insert
280     2 -10.242  120 -140  203 -204   imp:n=1         $ Lead
400     2 -10.242  140 -160  200 -204   imp:n=1         $ Lead
420    61 0.04284  120 -140  200 -201   imp:n=1         $ Fuel
440    63 0.04284  120 -140  201 -202   imp:n=1         $ Fuel
460    64 0.04284  120 -140  202 -203   imp:n=1         $ Fuel
999     0 -100:160:204                  imp:n=0         $ Void

100     pz -350.0
120     pz  -100.0
130     pz  -40.0
131     pz   15.0
132     pz   16.0
140     pz   100.0
160     pz  350.0
c
200     cz  25.0
201     cz  61.237
202     cz  82.916
203     cz 100.0
204     cz 400.0
c
421     cz  24.99

m2     82000.50c 0.445                    $ LBE, TD@400C=10.242 g/cc
       83209.50c 0.555
c
m20   40000.56c -0.0001 $ Croloy 1.25, from Maria and Ann-Louise
      12000.50c -0.0035
      6000.50c  -0.001
      25055.50c -0.004
      14000.50c -0.003
      24000.50c -0.0125
      42000.50c -0.006
      26000.55c -0.9699
c pwr1
m61     92238.50c  1.902E-04
        93237.55c  3.454E-05
        94238.50c  1.073E-05
        94239.55c  3.922E-04
        94240.50c  1.805E-04
        94241.50c  5.951E-05
```

```
        94242.50c  3.617E-05
        95241.50c  3.889E-05
        95242.50c  4.755E-08
        95243.50c  6.952E-06
        96243.35c  2.853E-08
        96244.50c  1.341E-06
        43099.50c  4.284E-04
        40000.56c  7.189E-03
        82000.50c  7.166E-03
        83209.50c  8.938E-03
        22000.50c  2.504E-05
        24000.50c  3.675E-03
        26000.50c  1.409E-02
        28000.50c  3.052E-03
        42000.50c  3.734E-04
c pwr2
m63     92238.50c  2.125E-04
        93237.55c  3.859E-05
        94238.50c  1.198E-05
        94239.55c  4.381E-04
        94240.50c  2.016E-04
        94241.50c  6.648E-05
        94242.50c  4.040E-05
        95241.50c  4.344E-05
        95242.50c  5.312E-08
        95243.50c  7.766E-06
        96243.35c  3.187E-08
        96244.50c  1.498E-06
        43099.50c  4.284E-04
        40000.56c  7.077E-03
        82000.50c  7.166E-03
        83209.50c  8.938E-03
        22000.50c  2.504E-05
        24000.50c  3.675E-03
        26000.50c  1.409E-02
        28000.50c  3.052E-03
        42000.50c  3.734E-04
print
tmp    6.032e-8 12r
c     Cell 141 is source
nps    2000
c
c    Source, d3=5 - evaporation spectrum, d1 gives parabolic
c    distribution with radius of 24.9 cm, d2 gives cubic dist
c    from -40 to 15 cm (top of target)
c
sdef  par=1  erg=d3  pos=0 0 -40  axs=0 0 1  rad=d1  ext=d2
sp1 -21 0.
si1  24.9
c sp2 -31 0.0667
sp2 -21 3.
si2 0. 54.99
sp3 -5
dbcn   12j 7.01e7
c pwr3
m64     92238.50c  2.279E-04
        93237.55c  4.139E-05
        94238.50c  1.285E-05
```

```
94239.55c  4.699E-04
94240.50c  2.162E-04
94241.50c  7.130E-05
94242.50c  4.334E-05
95241.50c  4.660E-05
95242.50c  5.698E-08
95243.50c  8.330E-06
96243.35c  3.419E-08
96244.50c  1.607E-06
43099.50c  4.284E-04
40000.56c  7.000E-03
82000.50c  7.166E-03
83209.50c  8.938E-03
22000.50c  2.504E-05
24000.50c  3.675E-03
26000.50c  1.409E-02
28000.50c  3.052E-03
42000.50c  3.734E-04
```

End of Appendix C

APPENDIX D - Monteburns Input File – test5.inp

```
adv1c  Advanced ATW, 2mDiamx2mHigh, 2 GW, 0.5mTarg, Equil, with Tc-99 in fuel
UNSU          ! Type of Operating System
3             ! Number of MCNP materials
61            ! MCNP Material number (must be less than 100)
63            ! MCNP Material number
64            ! MCNP Material number
0.            ! Material volume #1 (cc), input 0 to use mcnp value (if exists)
0.            ! Material volume #2
0.            ! Material volume #3
2000.         ! Power in MWt (for the entire system modeled in mcnp deck)
-200.         ! Recov. energy/fission (MeV); if negative use for U235, ratio other isos
0.            ! Total number of days burned (used if no feed)
4             ! Number of outer burn steps
40            ! Number of internal burn steps (multiple of 10)
1             ! Number of predictor steps (+1 on first step), 1 usually sufficient
0             ! Step number to restart after (0=beginning)
60            ! Number of origen2 library - next line is origen2 lib. location
/export/gus2/origen/libraries
.005          ! fractional importance (track isos with abs,fis,atom,mass fraction)
1             ! Intermediate keff calc. 0) No 1) Yes
14            ! Number of automatic tally isotopes, followed by list.
92238.50c
93237.55c
94238.50c
94239.55c
94240.50c
94241.50c
94242.50c
95241.50c
95242.50c
95243.50c
96242.50c
96243.35c
96244.50c
43099.50c
14
92238.50c
93237.55c
94238.50c
94239.55c
94240.50c
94241.50c
94242.50c
95241.50c
95242.50c
95243.50c
96242.50c
96243.35c
96244.50c
43099.50c
14
92238.50c
93237.55c
94238.50c
94239.55c
94240.50c
94241.50c
94242.50c
95241.50c
95242.50c
95243.50c
96242.50c
96243.35c
96244.50c
43099.50c
```

End of Appendix D

APPENDIX E - Feed Input File – test5.feed

```
Time   Days   Power MBMat Feed Begin&EndRates Remov. Fraction F.P.Removed
 Step Burned  Fract.  #   #      grams/day    Group#
   1  121.76  1.000   1   0     0.0     0.0     -1   0.990 !
                      2   0     0.0     0.0      0   0.000 !
                      3   0     0.0     0.0      0   0.000 !
   2  121.76  1.000   2   0     0.0     0.0     -1   0.990 !
                      3   0     0.0     0.0      0   0.000 !
                      1   1    -2.0  3300.0      0   0.000 !
   3  121.76  1.000   2   0     0.0     0.0     -1   0.990 !
                      3   0     0.0     0.0      0   0.000 !
                      1   1    -2.0  2900.0      0   0.000 !
   4  121.76  1.000   2   0     0.0     0.0     -1   0.990 !
                      3   0     0.0     0.0      0   0.000 !
                      1   1    -2.0  2650.0      0   0.000 !
   1                              ! # of feed specs
  13                              ! # isos in Feed #1, TC-99, LWR Discharge
43099  .055000
92238  .250000
93237  .044916
94238  .014001
94239  .514214
94240  .237591
94241  .078681
94242  .048014
95241  .051421
95242  .000068
95243  .009262
96243  .000034
96244  .001797
   1                              ! # of removal groups
   3                              ! # of ranges for Feed #1 removal step
 -10 -42                          ! 1st range for Feed #1
 -44 -79                          ! 2nd range for Feed #1
  92  92                          ! 3rd range for Feed #1
```

End of Appendix E

APPENDIX F - Sample MCNP Cross-section Map - mbxs.inp

```
 1001.50c
 1002.55c
 1003.50c
 2003.50c
 2004.50c
 3006.50c
 3007.55c
 4007.35c
 4009.50c
 5010.50c
 5011.56c
 6012.50c
 6013.35c
 6000.50c
 7014.50c
 7015.55c
 8016.50c
 9019.50c
11023.50c
12000.50c
13027.50c
14000.50c
15031.50c
16000.60c
16032.50c
17000.50c
18000.50c
19000.50c
20000.50c
21045.55c
22000.50c
23051.31c
23000.50c
24000.50c
25055.50c
26000.55c
27059.50c
28058.35c
28000.50c
29000.50c
31000.50c
33074.35c
33075.35c
35079.55c
35081.55c
36078.50c
36080.50c
36082.59c
36083.59c
36084.59c
36086.59c
37085.55c
37087.55c
39088.35c
39089.35c
40093.50c
```

```
40000.56c
41093.50c
42095.50c
42000.50c
43099.50c
44101.50c
44103.50c
45103.50c
45105.50c
46105.50c
46108.50c
47107.50c
47109.50c
47000.55c
48000.50c
50000.35c
53127.55c
53135.50c
54131.50c
54134.35c
54135.50c
54000.35c
55133.50c
55135.50c
56138.50c
59141.50c
60143.50c
60145.50c
60147.50c
60149.50c
61147.50c
61148.50c
61149.50c
62147.50c
62149.50c
62150.50c
62151.50c
62152.50c
63151.55c
63152.50c
63153.55c
63154.50c
63155.50c
63000.35c
64152.52c
64154.50c
64155.50c
64156.50c
64157.50c
64158.50c
64160.50c
64000.35c
67165.55c
69169.55c
72000.50c
73181.50c
74182.55c
74183.55c
```

```
74184.55c
74186.55c
74000.55c
75185.35c
75187.35c
77000.55c
78000.35c
79197.56c
82000.50c
83209.50c
90231.35c
90232.50c
90233.35c
91231.50c
91233.50c
92233.50c
92234.50c
92235.50c
92236.50c
92237.50c
92238.50c
92239.35c
92240.35c
93235.35c
93236.35c
93237.55c
93238.35c
94237.35c
94238.50c
94239.55c
94240.50c
94241.50c
94242.50c
94243.35c
95241.50c
95242.50c
95243.50c
96242.50c
96243.35c
96244.50c
96245.35c
96246.35c
96247.35c
96248.35c
97249.35c
98249.35c
98250.35c
98251.35c
98252.35c
```

End of Appendix F

End of Manual